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as of 14-Jan-2021

Agency Code:

Proposal Number: 63822EGMUR
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Agreement Number: W911NF-13-1-0390

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Final Report for Period Beginning 01-Sep-2013 and Ending 31-Aug-2018

Title: Information Engines_Nanoscale Control, Computing, and Communication out of Equilibrium

Begin Performance Period: 01-Sep-2013

End Performance Period: 31-Jul-2020

Report Term: 0-Other

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STEM Participants: 61

Major Goals: The Information Engines MURI's original goal was to develop a unified framework for understanding, designing, and implementing micron-scale and nanoscale information-processing engines and to provide the scientific foundation for future nanoscale devices with groundbreaking capabilities. These ambitious goals were met and, in several cases, exceeded as attested by the project's marked productivity; see <http://informationengines.org> ==> Research. These successes opened up a number of exciting future theoretical and experimental research avenues. The main efforts successfully developed methods to control nanoscale thermodynamic processes and, perhaps most importantly, culminated in successful detailed experimental tests and verifications of our theoretical results. That said, looking beyond this MURI, much remains to do and the core PI team continues to collaborate on and extend the Information Engines MURI's progress. Putting the accomplishments in broad perspective, let's briefly review the overall project goals.

Any given natural process can be viewed in two complementary and equally valid ways: First, as a "physical" system that is controlled by, manipulates, stores, and dissipates energy and, second, as a "dynamical" system that generates, stores, transforms, and destroys information. When considering it and its physical implementation as a unitary system, we see that information processing requires energy to drive it forward. An immediate result is that this energy is not completely transformed into processed information. Energy is dissipated. Such limitations dominate on the nanoscale, in particular, where fluctuations out of equilibrium are the rule and the distinction between organized and thermal energy, between heat and work, becomes ambiguous. The MURI's principle goal, therefore, was to find the physical limits of nanoscale information processing and control. To this end, the MURI pursued a set of interdependent tasks:

Task 1: Intrinsic Computation in Nanoscale Substrates: Develop concepts and mathematical tools that identify how dynamical processes store and transform information.

Task 2: Nonequilibrium Information Processing by Nanoscale Machines: Develop thermodynamic and statistical mechanical principles that govern the operation of information engines and then synthesize these with the tools of intrinsic computation from Task 1.

Task 3: Control and Optimization at the Nanoscale: Integrate methods of geometric optimal control theory and nonequilibrium statistical physics, instantiating the synthesis in concrete control problems posed by information engines.

Task 4: Validation: Optimal, Controllable Nanoscale Information Processing Agents: Develop experimental

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platforms with which to test the information-engines thermodynamic principles developed in Tasks 1, 2, and 3. These came to include nanoelectromechanical systems (NEMS) and flux qubits.

The long-term scientific challenges, implicit in Tasks 1 – 3, were not only to pioneer theoretical foundations, but to also establish a research community in information engines. Looking back over the MURI's seven-year extended existence, there are two notable accomplishments on this score. The first is the annual workshop series on Information Engines at the Frontiers of Nonequilibrium Thermodynamics, co-organized by the Lead PI, held each summer at the Telluride Science Research Center, and sponsored by ARO; except in 2020 due to the pandemic. In lieu of an in-person workshop the co-organizers and past participants are assembling a special issue on Thermodynamic Computing with Information Engines for the well-known Journal of Statistical Physics.

The second is that the MURI's successes catalyzed the emergence of information engines as signaling the dawn of a new era of thermodynamic computing or, as we have come to frame it, low-kBT computing. The initial experimental successes and rapidly-progressing theory led the Computing Community Consortium (CCC) in January 2019 to initiate a broad planning effort to develop this new paradigm—whose charge is to actively leverage and control inherent fluctuations in physical information-processing substrates (<https://cra.org/cce/events/thermodynamiccomputing/>). Note that in the 1990s and 2000s CCC was a key convener for research in quantum computing, among many other nascent information technologies. The current CCC effort is destined to play a similar guiding role for thermodynamic computing. Its report on Thermodynamic Computing is found at <https://arxiv.org/abs/1911.01968> and is uploaded with this Final Report. For those interested in delving further beyond this Final Report, we strongly recommend the CCC report as it paints a broad and bold picture of the path forward from this MURI.

Synopsis of Goals

The Information Engines MURI's led to major advances in controlling nanoscale thermodynamic systems and in determining the thermodynamic constraints on nanoscale information processing. In parallel, the MURI's flux-qubit information-engine devices were calibrated and extensively experimented on. The experimental results successfully validated key aspects of our theoretical predictions and led to new theoretical advances—e.g., the trajectory-class fluctuation theorems. The flux-qubit device was demonstrated to be markedly more appropriate for the project's goals than either the original molecular motor and NEMS systems. The following highlights our results.

A. Control of Nanoscale Thermodynamic Systems: Bringing together methods of geometric optimal control theory and nonequilibrium statistical physics, instantiated in concrete problems of designing working cycles for heat engines, has been a major goal of this part of the MURI project. The UCD-UMD teams focused on one of our three previously-developed approaches to controlling nanoscale thermodynamics systems: counterdiabatic control protocols for information processing tasks. Addressing very practical trade-offs in computing, counterdiabatic protocols provide finite-time “short-cuts” to, what otherwise are, adiabatic control protocols that require infinite time.

B. Principles of Information Thermodynamics: UCD determined the costs of thermodynamic controller's modular organization—the modularity dissipation—the first time thermodynamic costs have been associated with a system's structure and organization. This advances our suite of theoretical results to a design methodology for nanoscale devices with net positive thermodynamic benefit. And, critically, it laid the foundation (See Table I in the CCC report) for an extensive suite of experimental tests that continue on under other projects.

C. Nanoscale Information Engines Experiments: Due to key theoretical insights, the flux qubit became the main experimental focus. In the process, UCD-Caltech discovered new ways—called the trajectory-class fluctuation theorems—to diagnose success and failure modes of microscopic behaviors that support information processing using the mesoscopic “observable” of the distribution of works expended over a repeated protocol.

Overall, the MURI was remarkably productive with well over 100 peer-reviewed published articles. Most all are available through arXiv.org and the project website: <http://informationengines.org>. Importantly, 13 appeared in physics' top journals: 6 in Physical Review X and 7 in Physical Review Letters. Thus, the MURI's efforts were recognized at the highest levels and had substantial impact.

Administratively, the Information Engines MURI (#W911NF-18-1-0340) complements the Lead PI's ARO project Functional Pattern Formation in Thermodynamical Systems (#W911NF-18-1-0028). The latter started in 2018 and focuses on spatially-extended engines with the unique goal of tracking the flow of thermodynamic resources.

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Accomplishments: (Citation [XXX#] are in the Bibliography which is part of the uploaded, longer Final Report.)

PI Crooks: Continued his signature geometric approach to thermodynamic control and also contributed fundamental theoretical work on strongly coupled thermodynamic subsystems:

1. Thermodynamic geometry of minimum dissipation driven barrier crossing [GEC1].
2. Near optimal protocols in complex nonequilibrium transformations [GEC2].
3. Geometric approach to optimal nonequilibrium control [GEC3].

PI Crooks left the MURI Project during 2017 to develop a start-up company developing quantum machine learning.

PI Crutchfield: The computational mechanics of information processing in thermodynamic systems is close to complete:

- Functional fluctuations [JPC1]: Large deviation theory and computational mechanics predict how the thermodynamic functioning of information engines fluctuates in response to environmental behaviors.
- Costs of modularity [JPC3]: The modular architecture of an information engine comes at a thermodynamic cost, demonstrating that inefficiency arises from modularity by destroying the ability to leverage environmental correlations.
- Powerful mathematical and calculation methods [JPC5]: Introduced new methods are sufficiently powerful to yield closed-form analyses in many previously-intractable cases.
- Computational mechanics of infinite-memory processes [JPC6]: Extended the analysis of intrinsic computation to such infinite-state systems.
- Multivariate mutual information [JPC7,JPC16,JPC18]: A comprehensive software package in Python was developed and is available as open source.
- Toward quantum information engines [JPC8]: Crutchfield that quantum information engines exhibit a surprising array of new thermodynamic behaviors.
- The Principles of Requisite Complexity [JPC10]: For an adaptive system to take maximum thermodynamic advantage of its environment, it must be internally organized to represent its environment's correlations.
- Bacteria as environmental prediction engines [JPC11]: Crutchfield explained the role of bacterial epigenetics as coding predictive ("causal") states of the environment.
- Causal asymmetry in a quantum world [JPC12]: Crutchfield showed that quantum structural complexity is time symmetric, raising fundamental issues about the origins of asymmetry in classical physics and so in thermodynamic information processing.
- Spacetime computational mechanics [JPC13]: This effort laid out the theoretical foundations for structure and causality in spacetime.
- Information theory software package [JPC17]: Open source Python library for discrete information theory.
- Fraudulent white noise [JPC18]: Crutchfield gave a new view of "unstructured" and "uncorrelated" processes that goes some distance to disabuse us of misinterpreting or even simply dismissing structure present in apparently-noisy observations.
- Information engine performance [JPC19]: Crutchfield developed new error-dissipation trade-offs in information engines controlled via time-symmetric protocols.
- Measurement-induced randomness and structure [JPC20]: Crutchfield developed close parallels and distinctions between quantum and classical physics in terms of randomness and structure that measurement can generate or remove.

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- Harnessing fluctuations in thermodynamic computing [JPC21]: Crutchfield developed mesoscopic methods to track successful and failed microscopic information processing.
- Shortcuts to thermodynamic computing [JPC22]: Crutchfield and Jarzynski developed new counterdiabatic control methods that give much advantage in thermodynamic control.

PI DeWeese: Developed new approaches for understanding and controlling nonequilibrium systems and applied these insights to network theory, learning, engineered systems, and fundamental physics problems. DeWeese generalized the geometric framework for finding minimum dissipation protocols to include a systematic expansion of all terms beyond the second-order equations known previously, as well as a generalization of the “escorted dynamics” framework for transitioning the full distribution of a thermodynamic system from one state to another in finite time to the case of more than one control parameter [MRD1,MRD2,MRD3].

PI Jarzynski: Continued to pioneer novel control strategies for classical and quantum thermodynamic systems.

Thermodynamics of periodically-driven systems: Jarzynski showed for discrete-state Markov dynamics that such stochastic pumps—periodically driven stochastic systems—are able to mimic nonequilibrium steady states [CJ5] and extended this to diffusive motion in one degree of freedom [CJ1].

Programmable Maxwell's Demon: Jarzynski developed a mechanistic model of a programmable Maxwell's Demon [CJ2] that, interacting with a thermal bath, can raise a mass that against gravity.

Second Law violations: Jarzynski showed that it is possible, in principle, to design protocols in which most realizations give rise to Second Law violations [CJ3].

Shortcuts to adiabaticity: Jarzynski developed methods to construct shortcuts for a variety of systems—classical, quantum, and stochastic [CJ6].

Counterdiabatic erasure: Crutchfield and Jarzynski applied this to bit erasure [JPC22].

Quantum adiabatic control: For quantum systems, Jarzynski constructed local shortcuts to adiabaticity that rapidly drive a system from an excited state of an initial Hamiltonian to the corresponding state of the final Hamiltonian [CJ4].

PI Krishnaprasad: Developed approaches to control nonequilibrium processes, applying them to thermodynamic computation, collective motion, population dynamics, and interface growth.

1. Thermodynamic efficiency in a stochastic dissipative oscillator [PSK1]: Solved the design problem of a cyclic protocol (heat engine) that extracts a prescribed amount of work with maximal thermodynamic efficiency in a stochastic dissipative system.
2. Subriemannian geometry in collective motion [PSK3,PSK4,PSK5]: Extended collective subriemannian geometry to continuum settings with long-range propagation of information in collectives.
3. Population games and their control [PSK2,PSK4,PSK7]: Population games and their control formulated a variational principle for replicator.
4. Controlling KPZ interface growth [PSK6]: Control of the KPZ equation of interface growth via variance minimization problem.

PI Roukes: Roukes' Caltech team demonstrated that superconducting flux qubits can act as nanoscale switches displaying strong fluctuations at low temperatures. In particular, the flux qubits were validated as ideal classical double-well systems at temperatures near 500 mK. In collaboration with the UC Davis team, functional partitions within an erasure protocol were experimentally verified using the flux qubit [JPC21,MR1]. To monitor the thermodynamics, Caltech measured thermal conductance of suspended superconducting-normal-superconducting (SNS) thermometers and found a strong reduction of thermal conductance necessary for the thermodynamic measurements of information processing in flux qubits. Combining the SNS junction thermometers with the flux qubits on the same chip is underway in collaboration with Siyuan Han (University of Kansas). Roukes' Caltech team designed the flux qubit/SNS thermometer chip and reconfiguring the measurement equipment for

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thermodynamic measurements of operations within the flux qubit.

PI Hess: Explored how velocity fluctuations in microtubule transport by surface-adhered kinesin motors revealed key insights on how the degree of velocity fluctuations directly relates to a loss in efficiency and on how heterogeneity in motor attachment geometry and the anharmonicity in the tail stiffness conspire to dominate the velocity fluctuations at high motor densities. His Columbia University team left the MURI project during Fall 2016.

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Training Opportunities: The Information Engine MURI training effort was substantial with an average of half a dozen postdoctoral and two dozen graduate researchers, with 20 PhDs granted.

2019: 7 postdoctoral researchers, 18 graduate student researchers, and an undergraduate research intern. Five PhD degrees.

2018: 8 postdoctoral researchers, 20 graduate student researchers, and several undergraduate research interns. Three PhD degrees.

2017: 7 postdoctoral researchers, 20 graduate student researchers, and several undergraduate research interns. Six PhD degrees.

2016: 7 postdoctoral researchers, 29 graduate student researchers, and several undergraduate research interns. Five PhD degrees, one MS degree.

Ph.D. Degrees Earned

- Cina Aghamohammadi: “Memory and Thermodynamic Costs of Sampling and Biased Sampling”, Ph.D. Dissertation in Physics, University of California at Davis, August 2018.
- Mayur Mudigonda, “Inference algorithms and sensorimotor representations in brains and machines”, PhD dissertation in Vision Science, University of California at Berkeley, June 2019.
- Udit Halder: “Optimality, Synthesis and a Continuum Model for Collective Motion”, Ph.D. in Engineering, University of Maryland, College Park, April 2019.
- Vidya Radu: “Collective Behavior, Information Propagation, and Noise”, Ph.D. in Engineering, University of Maryland, College Park, May 2019.
- Eric Dodds: “Statistical learning models of sensory processing and implications of biological constraints”, PhD dissertation in Physics, December 2018.
- Alexander Boyd: “Thermodynamics of Correlations and Structure in Information Engines”, Ph.D. Dissertation in Physics, University of California at Davis, December 2017.
- Ayoti Patra, “Bridging quantum, classical and stochastic shortcuts to adiabaticity”, PhD in Physics, University of Maryland, College Park, September 2017.
- Y. Huang: “Optimal control of heat engines in non-equilibrium statistical mechanics”, PhD in Engineering; August 2017.
- Nix Barnett: “Mechanisms within the Black Box: Prediction, Computation, Randomness, and Complexity of Input-Output Processes via the χ^2 -Transducer”, PhD in Mathematics, University of California, Davis, August 2016.
- Sarah E. Marzen: “Bio-inspired Problems in Rate-distortion Theory”, PhD in Physics, University of California, Berkeley, August 2016. Now, Physics of Living System Fellow with Prof. Jeremy England, Physics, MIT.
- Paul Riechers: “Exact Results Regarding the Physics of Complex Systems via Linear Algebra, Hidden Markov Models, and Information Theory”, Ph.D. Dissertation in Physics, University of California at Davis, December 2016.
- J. Demers, “Stochastic processes in physics: deterministic origins and controls”, PhD in Physics, University of Maryland, College Park, December 2016. Dr. Demers is now a postdoc in Prof. William Fagan’s group in the Department of Biology, University of Maryland, College Park.
- Amy T-C. Lam, “Assembly in Dynamic Nanoscale Systems”, PhD in Biomedical Engineering, Columbia University, New York, December 2015.
- Zhiyue Lu: “Topics in equilibrium and nonequilibrium thermodynamics: computing crystalline free energies and engineering Maxwell’s demon”, PhD in Chemical Physics, University of Maryland, College Park, December 2015.

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- Biswadip Dey (UMD, 2014); Now, Postdoctoral Fellow in Mech & Aero Eng, Princeton University.
- Patrick Zulkowski (UCB, 2014) “The Geometry of Thermodynamic Control”; Now, Assistant Professor, Berkeley City College.
- Ofer Idan (Columbia, 2014) “Modeling Nanoscale Transport Systems”.
- Nick Travers (UCD, 2014); Now, Asst. Prof, Mathematics, University of Indiana, Bloomington.
- Ryan G. James (Physics, UC Davis) Ph.D. August 2013.
- Nicholas F. Travers (Mathematics, UC Davis) Ph.D. August 2013.

M.S. Degrees Earned During Reporting Period

- K. Miltenberger, MS thesis on collective behavior. April 2016.

Additional information on programs, students, and faculty of the Information Engines MURI project and the Complexity Sciences Center is available online at <http://informationengines.org/> and <http://csc.ucdavis.edu/>, respectively.

Results Dissemination: The Information Engines MURI’s productivity was sustained at a high level, indicating an intellectual maturation as the teams overcame previous theoretical and experimental challenges. The results were disseminated rather widely. Annual summary:

2019: Thirty-eight manuscripts were in play, 19 appeared in peer-reviewed, high-profile journals, another 11 manuscripts were under review, and 8 were in preparation.

2018: 40 manuscripts, 25 appeared in peer-reviewed, high-profile journals and another 11 manuscripts under review.

2017: 52 manuscripts, 35 appeared in peer-reviewed, high-profile journals and another 17 manuscripts were under review.

2016: 40 manuscripts, 24 appeared in peer-reviewed, high-profile journals and another 21 manuscripts were submitted.

Each year during the MURI, the Lead PI co-organized the workshop on Information Engines at the Frontier of Nanoscale Thermodynamics, held at the Telluride Science Research Center, typically 10 days during July, and supported by ARO. The Lead PI also organized Beyond Shannon—The Structure and Meaning of Information, held at the Institute for Advanced Study, University of Amsterdam, 6-8 May 2019.

Space does not permit listing the hundreds of presentations—team colloquia, keynotes, lecture courses, invited presentations, and team-organized meetings and workshops. These are, however, documented in detail in the annual Interim Progress Reports.

Honors and Awards: Space does not permit listing the many dozens of PI honors, awards, and appointments. These are, however, documented in detail in the annual Interim Progress Reports.

Protocol Activity Status:

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Technology Transfer: • PI Crutchfield: Continues to maintain and augment the MURI's website <http://informationengines.org/> to facilitate team collaborations and outreach.

- PI Crutchfield: Continues to develop the open source Python package "Computational Mechanics in Python" (CMPy) consisting of most of computational mechanics' constructive mathematical results and methods. Jupyter/Python notebooks continue to be developed to illustrate calculational details reported in our publications. A suite of over two-dozen Jupyter notebooks was developed as tutorials. CMPy has been ported to run on the Jupyter notebook service CoCalc.com. Efforts initiated to port CMPy from Python 2.7.X to Python 3.X.
- PI Crutchfield: Further developed the open source Discrete Information Theory Python package dit: <https://github.com/dit/dit>. Most notably, it was extended to include an even more complete suite of multivariate information measures for dynamical and stochastic networks. Including, in particular, new algorithms for secret key agreement measures of unique information [JPC17].
- PI Krishnaprasad: Transfer of knowledge to the Naval Research Laboratory through collaboration with Dr. Eric Justh has continued on a regular basis. Concrete applications of this transfer effort are expected in the area of collective behavior in unmanned aerial and marine systems. Other applications to development of machine learning algorithms are also under consideration.
- PI Krishnaprasad: There have been multiple interactions with Dr. Adam Svenkeson (Research Scientist at Army Research Laboratory, Aberdeen, MD) and these are expected to continue on a monthly basis, with the aim of developing collaborations.
- PI Krishnaprasad: Additional collaboration with Northrop Grumman Mission Systems (contact: Dr. Isidoros Doxas) has been initiated to allow further developments in the direction of adversarial learning modeled by controlled replicator dynamics subject to noise. Applications are being considered in agile surveillance systems capable of countering adversarial responses. PI Krishnaprasad will present new results at a Northrop Grumman Research Symposium in October 2019.
- PI Krishnaprasad: A new collaboration, including joint proposal development has been initiated with Ford in the area of autonomous systems and machine learning.

PARTICIPANTS:

Participant Type: PD/PI

Participant: James P Crutchfield

Person Months Worked: 3.00

Project Contribution:

International Collaboration:

International Travel:

National Academy Member: N

Other Collaborators:

Funding Support:

Participant Type: Co-Investigator

Participant: Gavin Crooks

Person Months Worked: 1.00

Project Contribution:

International Collaboration:

International Travel:

National Academy Member: N

Other Collaborators:

Funding Support:

Participant Type: Co-Investigator

Participant: Micheal DeWeese

Person Months Worked: 1.00

Project Contribution:

International Collaboration:

Funding Support:

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International Travel:
National Academy Member: N
Other Collaborators:

Participant Type: Co-Investigator

Participant: Henry Hess

Person Months Worked: 1.00

Project Contribution:

International Collaboration:

International Travel:

National Academy Member: N

Other Collaborators:

Funding Support:

Participant Type: Co-Investigator

Participant: Christopher Jarzynski

Person Months Worked: 1.00

Project Contribution:

International Collaboration:

International Travel:

National Academy Member: N

Other Collaborators:

Funding Support:

Participant Type: Co-Investigator

Participant: P. S. Krishnaprasad

Person Months Worked: 1.00

Project Contribution:

International Collaboration:

International Travel:

National Academy Member: N

Other Collaborators:

Funding Support:

Participant Type: Co-Investigator

Participant: Michael L Roukes

Person Months Worked: 1.00

Project Contribution:

International Collaboration:

International Travel:

National Academy Member: N

Other Collaborators:

Funding Support:

Participant Type: Staff Scientist (doctoral level)

Participant: Warren Fon

Person Months Worked: 4.00

Project Contribution:

International Collaboration:

International Travel:

National Academy Member: N

Other Collaborators:

Funding Support:

Participant Type: Staff Scientist (doctoral level)

Participant: Matthew Matheny

Person Months Worked: 5.00

Project Contribution:

Funding Support:

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International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Participant Type: Staff Scientist (doctoral level)

Participant: Korana Burke

Person Months Worked: 1.00

Funding Support:

Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Participant Type: Staff Scientist (doctoral level)

Participant: John Mahoney

Person Months Worked: 1.00

Funding Support:

Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Participant Type: Staff Scientist (doctoral level)

Participant: Dowman Varn

Person Months Worked: 1.00

Funding Support:

Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Participant Type: Postdoctoral (scholar, fellow or other postdoctoral position)

Participant: Fabio Anza

Person Months Worked: 1.00

Funding Support:

Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Participant Type: Postdoctoral (scholar, fellow or other postdoctoral position)

Participant: Alexander Boyd

Person Months Worked: 1.00

Funding Support:

Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Participant Type: Postdoctoral (scholar, fellow or other postdoctoral position)

Participant: Ryan James

Person Months Worked: 4.00

Funding Support:

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Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Participant Type: Postdoctoral (scholar, fellow or other postdoctoral position)

Participant: Sarah Marzen

Person Months Worked: 1.00

Funding Support:

Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Participant Type: Postdoctoral (scholar, fellow or other postdoctoral position)

Participant: Paul Riechers

Person Months Worked: 1.00

Funding Support:

Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Participant Type: Postdoctoral (scholar, fellow or other postdoctoral position)

Participant: Olli-Pentti Saira

Person Months Worked: 4.00

Funding Support:

Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Participant Type: Postdoctoral (scholar, fellow or other postdoctoral position)

Participant: Cina Aghamohammadi

Person Months Worked: 1.00

Funding Support:

Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Participant Type: Postdoctoral (scholar, fellow or other postdoctoral position)

Participant: Louis Kang

Person Months Worked: 1.00

Funding Support:

Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Participant Type: Postdoctoral (scholar, fellow or other postdoctoral position)

Participant: Dibyendu Mandal

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Person Months Worked: 10.00

Funding Support:

Project Contribution:

International Collaboration:

International Travel:

National Academy Member: N

Other Collaborators:

Participant Type: Postdoctoral (scholar, fellow or other postdoctoral position)

Participant: Jascha Sohl-Dickstein

Person Months Worked: 2.00

Funding Support:

Project Contribution:

International Collaboration:

International Travel:

National Academy Member: N

Other Collaborators:

Participant Type: Postdoctoral (scholar, fellow or other postdoctoral position)

Participant: John Mahoney

Person Months Worked: 1.00

Funding Support:

Project Contribution:

International Collaboration:

International Travel:

National Academy Member: N

Other Collaborators:

Participant Type: Postdoctoral (scholar, fellow or other postdoctoral position)

Participant: Parag Katira

Person Months Worked: 1.00

Funding Support:

Project Contribution:

International Collaboration:

International Travel:

National Academy Member: N

Other Collaborators:

Participant Type: Postdoctoral (scholar, fellow or other postdoctoral position)

Participant: Patrick Zulkowski

Person Months Worked: 6.00

Funding Support:

Project Contribution:

International Collaboration:

International Travel:

National Academy Member: N

Other Collaborators:

Participant Type: Postdoctoral (scholar, fellow or other postdoctoral position)

Participant: Sebastian Deffner

Person Months Worked: 1.00

Funding Support:

Project Contribution:

International Collaboration:

International Travel:

National Academy Member: N

Other Collaborators:

Participant Type: Graduate Student (research assistant)

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Participant: Jeffrey Emenheiser

Person Months Worked: 1.00

Funding Support:

Project Contribution:

International Collaboration:

International Travel:

National Academy Member: N

Other Collaborators:

Participant Type: Graduate Student (research assistant)

Participant: David Gier

Person Months Worked: 1.00

Funding Support:

Project Contribution:

International Collaboration:

International Travel:

National Academy Member: N

Other Collaborators:

Participant Type: Graduate Student (research assistant)

Participant: Wade Hodson

Person Months Worked: 6.00

Funding Support:

Project Contribution:

International Collaboration:

International Travel:

National Academy Member: N

Other Collaborators:

Participant Type: Graduate Student (research assistant)

Participant: Xincheng Li

Person Months Worked: 12.00

Funding Support:

Project Contribution:

International Collaboration:

International Travel:

National Academy Member: N

Other Collaborators:

Participant Type: Graduate Student (research assistant)

Participant: Alexandra Jurgens

Person Months Worked: 3.00

Funding Support:

Project Contribution:

International Collaboration:

International Travel:

National Academy Member: N

Other Collaborators:

Participant Type: Graduate Student (research assistant)

Participant: Raj Katti

Person Months Worked: 2.00

Funding Support:

Project Contribution:

International Collaboration:

International Travel:

National Academy Member: N

Other Collaborators:

RPPR Final Report
as of 14-Jan-2021

Participant Type: Graduate Student (research assistant)

Participant: Xincheng Lei

Person Months Worked: 6.00

Funding Support:

Project Contribution:

International Collaboration:

International Travel:

National Academy Member: N

Other Collaborators:

Participant Type: Graduate Student (research assistant)

Participant: Samuel Loomis

Person Months Worked: 4.00

Funding Support:

Project Contribution:

International Collaboration:

International Travel:

National Academy Member: N

Other Collaborators:

Participant Type: Graduate Student (research assistant)

Participant: Daniella Masante

Person Months Worked: 1.00

Funding Support:

Project Contribution:

International Collaboration:

International Travel:

National Academy Member: N

Other Collaborators:

Participant Type: Graduate Student (research assistant)

Participant: Adam Rupe

Person Months Worked: 4.00

Funding Support:

Project Contribution:

International Collaboration:

International Travel:

National Academy Member: N

Other Collaborators:

Participant Type: Graduate Student (research assistant)

Participant: Pratik Sachdeva

Person Months Worked: 1.00

Funding Support:

Project Contribution:

International Collaboration:

International Travel:

National Academy Member: N

Other Collaborators:

Participant Type: Graduate Student (research assistant)

Participant: Ariadna Venegas-Li

Person Months Worked: 3.00

Funding Support:

Project Contribution:

International Collaboration:

International Travel:

National Academy Member: N

Other Collaborators:

RPPR Final Report
as of 14-Jan-2021

Participant Type: Graduate Student (research assistant)

Participant: Kyle Ray

Person Months Worked: 6.00

Funding Support:

Project Contribution:

International Collaboration:

International Travel:

National Academy Member: N

Other Collaborators:

Participant Type: Graduate Student (research assistant)

Participant: Neha Wadia

Person Months Worked: 1.00

Funding Support:

Project Contribution:

International Collaboration:

International Travel:

National Academy Member: N

Other Collaborators:

Participant Type: Graduate Student (research assistant)

Participant: Greg Wimsatt

Person Months Worked: 12.00

Funding Support:

Project Contribution:

International Collaboration:

International Travel:

National Academy Member: N

Other Collaborators:

Participant Type: Graduate Student (research assistant)

Participant: Ryan Zarcone

Person Months Worked: 1.00

Funding Support:

Project Contribution:

International Collaboration:

International Travel:

National Academy Member: N

Other Collaborators:

Participant Type: Graduate Student (research assistant)

Participant: Michael Fang

Person Months Worked: 1.00

Funding Support:

Project Contribution:

International Collaboration:

International Travel:

National Academy Member: N

Other Collaborators:

Participant Type: Graduate Student (research assistant)

Participant: Andrew Ligeralde

Person Months Worked: 1.00

Funding Support:

Project Contribution:

International Collaboration:

International Travel:

National Academy Member: N

Other Collaborators:

RPPR Final Report
as of 14-Jan-2021

Participant Type: Graduate Student (research assistant)

Participant: Charles Frye

Person Months Worked: 1.00

Funding Support:

Project Contribution:

International Collaboration:

International Travel:

National Academy Member: N

Other Collaborators:

Participant Type: Graduate Student (research assistant)

Participant: Steven Lee

Person Months Worked: 1.00

Funding Support:

Project Contribution:

International Collaboration:

International Travel:

National Academy Member: N

Other Collaborators:

Participant Type: Graduate Student (research assistant)

Participant: Mayur Mudigonda

Person Months Worked: 1.00

Funding Support:

Project Contribution:

International Collaboration:

International Travel:

National Academy Member: N

Other Collaborators:

Participant Type: Graduate Student (research assistant)

Participant: Tyler Maltba

Person Months Worked: 1.00

Funding Support:

Project Contribution:

International Collaboration:

International Travel:

National Academy Member: N

Other Collaborators:

Participant Type: Graduate Student (research assistant)

Participant: Nick CinkoAdam Frim

Person Months Worked: 1.00

Funding Support:

Project Contribution:

International Collaboration:

International Travel:

National Academy Member: N

Other Collaborators:

Participant Type: Graduate Student (research assistant)

Participant: Eric Dodds

Person Months Worked: 1.00

Funding Support:

Project Contribution:

International Collaboration:

International Travel:

National Academy Member: N

RPPR Final Report
as of 14-Jan-2021

Other Collaborators:

Participant Type: Graduate Student (research assistant)

Participant: Cina Aghamohammadi

Person Months Worked: 6.00

Funding Support:

Project Contribution:

International Collaboration:

International Travel:

National Academy Member: N

Other Collaborators:

Participant Type: Graduate Student (research assistant)

Participant: Alexander Boyd

Person Months Worked: 6.00

Funding Support:

Project Contribution:

International Collaboration:

International Travel:

National Academy Member: N

Other Collaborators:

Participant Type: Graduate Student (research assistant)

Participant: Udit Halder

Person Months Worked: 1.00

Funding Support:

Project Contribution:

International Collaboration:

International Travel:

National Academy Member: N

Other Collaborators:

Participant Type: Graduate Student (research assistant)

Participant: Yunlong Huang

Person Months Worked: 12.00

Funding Support:

Project Contribution:

International Collaboration:

International Travel:

National Academy Member: N

Other Collaborators:

Participant Type: Graduate Student (research assistant)

Participant: Katherine Klymko

Person Months Worked: 1.00

Funding Support:

Project Contribution:

International Collaboration:

International Travel:

National Academy Member: N

Other Collaborators:

Participant Type: Graduate Student (research assistant)

Participant: Vidya Radu

Person Months Worked: 6.00

Funding Support:

Project Contribution:

International Collaboration:

International Travel:

RPPR Final Report
as of 14-Jan-2021

National Academy Member: N
Other Collaborators:

Participant Type: Graduate Student (research assistant)

Participant: Andrew Mavin Smith

Person Months Worked: 1.00

Funding Support:

Project Contribution:

International Collaboration:

International Travel:

National Academy Member: N

Other Collaborators:

Participant Type: Graduate Student (research assistant)

Participant: Joseph Demers

Person Months Worked: 6.00

Funding Support:

Project Contribution:

International Collaboration:

International Travel:

National Academy Member: N

Other Collaborators:

Participant Type: Graduate Student (research assistant)

Participant: Nix Barnett

Person Months Worked: 6.00

Funding Support:

Project Contribution:

International Collaboration:

International Travel:

National Academy Member: N

Other Collaborators:

Participant Type: Graduate Student (research assistant)

Participant: Paul Riechers

Person Months Worked: 6.00

Funding Support:

Project Contribution:

International Collaboration:

International Travel:

National Academy Member: N

Other Collaborators:

Participant Type: Graduate Student (research assistant)

Participant: Dmitry Shemetov

Person Months Worked: 1.00

Funding Support:

Project Contribution:

International Collaboration:

International Travel:

National Academy Member: N

Other Collaborators:

Participant Type: Graduate Student (research assistant)

Participant: Henri Palacci

Person Months Worked: 6.00

Funding Support:

Project Contribution:

International Collaboration:

RPPR Final Report
as of 14-Jan-2021

International Travel:
National Academy Member: N
Other Collaborators:

Participant Type: Graduate Student (research assistant)

Participant: V. Raju

Person Months Worked: 1.00

Funding Support:

Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Participant Type: Graduate Student (research assistant)

Participant: Michael Prijatelj

Person Months Worked: 1.00

Funding Support:

Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Participant Type: Graduate Student (research assistant)

Participant: Megan Armstrong

Person Months Worked: 3.00

Funding Support:

Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Participant Type: Graduate Student (research assistant)

Participant: Ofer Idan

Person Months Worked: 4.00

Funding Support:

Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Participant Type: Graduate Student (research assistant)

Participant: Amy Lam

Person Months Worked: 5.00

Funding Support:

Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Participant Type: Graduate Student (research assistant)

Participant: Ayoti Patri

Person Months Worked: 6.00

Funding Support:

Project Contribution:

RPPR Final Report
as of 14-Jan-2021

International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Participant Type: Graduate Student (research assistant)

Participant: Zhiyue Lu

Person Months Worked: 6.00

Funding Support:

Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Participant Type: Graduate Student (research assistant)

Participant: Biswadip Dey

Person Months Worked: 1.00

Funding Support:

Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Participant Type: Graduate Student (research assistant)

Participant: Patrick Zulkowski

Person Months Worked: 6.00

Funding Support:

Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Participant Type: Graduate Student (research assistant)

Participant: Pooneh Ara

Person Months Worked: 2.00

Funding Support:

Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Participant Type: Graduate Student (research assistant)

Participant: Benny Brown

Person Months Worked: 1.00

Funding Support:

Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Participant Type: Graduate Student (research assistant)

Participant: Sarah Marzen

Person Months Worked: 1.00

Funding Support:

RPPR Final Report
as of 14-Jan-2021

Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Participant Type: Graduate Student (research assistant)

Participant: Grant Rotskoff

Person Months Worked: 1.00

Funding Support:

Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Participant Type: Graduate Student (research assistant)

Participant: K. Miltenberger

Person Months Worked: 6.00

Funding Support:

Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Participant Type: Graduate Student (research assistant)

Participant: Neda Bassir Kazeruni

Person Months Worked: 3.00

Funding Support:

Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Participant Type: Graduate Student (research assistant)

Participant: Stanislav Tsitkov

Person Months Worked: 3.00

Funding Support:

Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Participant Type: Undergraduate Student

Participant: Sara Pohland

Person Months Worked: 1.00

Funding Support:

Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Participant Type: Undergraduate Student

Participant: Hyun Su Kim

RPPR Final Report
as of 14-Jan-2021

Person Months Worked: 1.00

Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Funding Support:

Participant Type: Undergraduate Student

Participant: Bahti Zakirov

Person Months Worked: 1.00

Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Funding Support:

Participant Type: Undergraduate Student

Participant: Joshua Ruebeck

Person Months Worked: 1.00

Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Funding Support:

Participant Type: Undergraduate Student

Participant: Brent Schlotfeldt

Person Months Worked: 1.00

Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Funding Support:

Participant Type: Undergraduate Student

Participant: Alexandra Nilles

Person Months Worked: 1.00

Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Funding Support:

Participant Type: Undergraduate Student

Participant: Andrew Berger

Person Months Worked: 1.00

Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Funding Support:

Participant Type: Undergraduate Student

RPPR Final Report

as of 14-Jan-2021

Participant: Brendan Roberts
Person Months Worked: 1.00
Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Funding Support:

ARTICLES:

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published

Journal: Physics Letters A

Publication Identifier Type: DOI

Publication Identifier: 10.1016/j.physleta.2014.05.014

Volume: 378

Issue: 0

First Page #: 0

Date Submitted: 8/29/16 12:00AM

Date Published:

Publication Location:

Article Title: Chaos forgets and remembers: Measuring information creation, destruction, and storage

Authors: Ryan G. James, Korana Burke, James P. Crutchfield

Keywords: chaos, entropy rate, bound information, Shannon information measures, information diagram, Tent map, Logistic map, Lozi map

Abstract: The hallmark of deterministic chaos is that it creates information—the rate being given by the Kolmogorov–Sinai metric entropy. Since its introduction half a century ago, the metric entropy has been used as a unitary quantity to measure a system’s intrinsic unpredictability. Here, we show that it naturally decomposes into two structurally meaningful components: A portion of the created information—the ephemeral information—is forgotten and a portion—the bound information—is remembered. The bound information is a new kind of intrinsic computation that differs fundamentally from information creation: it measures the rate of active information storage. We show that it can be directly and accurately calculated via symbolic dynamics, revealing a hitherto unknown richness in how dynamical systems compute.

Distribution Statement: 3-Distribution authorized to U.S. Government Agencies and their contractors

Acknowledged Federal Support: Y

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published

Journal: Entropy

Publication Identifier Type: DOI

Publication Identifier: 10.3390/e16094713

Volume: 16

Issue: 9

First Page #: 0

Date Submitted:

Date Published:

Publication Location:

Article Title: Information Anatomy of Stochastic Equilibria

Authors:

Keywords: Langevin equation; entropy rate; ephemeral information; bound information; time-local predictive information

Abstract: A stochastic nonlinear dynamical system generates information, as measured by its entropy rate. Some—the ephemeral information—is dissipated and some—the bound information—is actively stored and so affects future behavior. We derive analytic expressions for the ephemeral and bound information in the limit of infinitesimal time discretization for two classical systems that exhibit dynamical equilibria: first-order Langevin equations (i) where the drift is the gradient of an analytic potential function and the diffusion matrix is invertible and (ii) with a linear drift term (Ornstein–Uhlenbeck), but a noninvertible diffusion matrix. In both cases, the bound information is sensitive to the drift and diffusion, while the ephemeral information is sensitive only to the diffusion matrix and not to the drift. Notably, this information anatomy changes discontinuously as any of the diffusion coefficients vanishes, indicating that it is very sensitive to the noise structure. We then calc

Distribution Statement: 1-Approved for public release; distribution is unlimited.

Acknowledged Federal Support:

RPPR Final Report as of 14-Jan-2021

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published

Journal: WIREs Computational Statistics

Publication Identifier Type: Publication Identifier:

Volume: 6 Issue: 2 First Page #: 75

Date Submitted: Date Published:

Publication Location:

Article Title: The dreams of theory

Authors:

Keywords: computational science; complex systems; artificial science; Big Data; Big Iron

Abstract: Computing power and sophisticated data acquisition mask the fact that, in many sciences and engineering, the balance between theory and experiment is getting increasingly out of whack. The imbalance becomes an even greater concern in light of the increasingly complex natural systems science now confronts and the increasingly complex and interdependent sociotechnical systems modern engineering allows us to construct. Given its critical role in understanding such complex systems, Big Theory deserves a place alongside Big Data and Big Iron, says Jim Crutchfield.

Distribution Statement: 1-Approved for public release; distribution is unlimited.

Acknowledged Federal Support:

Publication Type: Journal Article Peer Reviewed: N **Publication Status:** 1-Published

Journal: Cosyne 2015

Publication Identifier Type: Publication Identifier:

Volume: 0 Issue: 0 First Page #: 0

Date Submitted: 8/26/17 12:00AM Date Published:

Publication Location:

Article Title: Statistical complexity of neural spike trains

Authors: Sarah E. Marzen, Michael DeWeese, James P. Crutchfield

Keywords: information, entropy rate, statistical complexity, excess entropy, integrate and fire neuron

Abstract: We present closed-form expressions for the entropy rate, statistical complexity, and predictive information for the spike train of a single neuron in terms of the first passage time probability distribution. Our analysis applies to any one-dimensional neural model where observation of a spike causes the neuron to "reset" to some membrane voltage and in which any noise term is uncorrelated in time. We then use these formulae to study the linear leaky integrate-and-fire and quadratic integrate-and-fire neurons driven by white noise in the naturally spiking regime. The statistical complexity is simply related to the interspike interval's mean and coefficient of variation. The excess entropy, or the total predictive information, is highest for neural spike trains with low interspike interval coefficients of variation. Both the statistical complexity and the excess entropy arise naturally in the context of predictive rate-distortion and could be useful for characterizing ...

Distribution Statement: 3-Distribution authorized to U.S. Government Agencies and their contractors

Acknowledged Federal Support: Y

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published

Journal: arxiv.org:1407.7159 [cond-mat]

Publication Identifier Type: Publication Identifier: 10.1107/S2053273315005264

Volume: A71 Issue: 0 First Page #: 423

Date Submitted: 8/29/16 12:00AM Date Published: 3/14/15 7:00AM

Publication Location:

Article Title: Pairwise Correlations in Layered Close-Packed Structures

Authors: P. M. Riechers, D. P. Varn, J. P. Crutchfield

Keywords: X-ray diffraction, planar disorder, stacking fault, z-transform, spectral decomposition, pair distribution function

Abstract: Given a description of the stacking statistics of layered close-packed structures in the form of a hidden Markov model, analytical expressions are developed for the pairwise correlation functions between the layers. These may be calculated analytically as explicit functions of model parameters or the expressions may be used as a fast, accurate and efficient way to obtain numerical values. Several examples are presented, finding agreement with previous work as well as deriving new relations.

Distribution Statement: 3-Distribution authorized to U.S. Government Agencies and their contractors

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as of 14-Jan-2021

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published

Journal: Physics Letters A

Publication Identifier Type: DOI

Publication Identifier: 10.1016/j.physleta.2016.01.008

Volume: 380

Issue: 0

First Page #: 998

Date Submitted: 8/26/17 12:00AM

Date Published:

Publication Location:

Article Title: Exact Complexity: The Spectral Decomposition of Intrinsic Computation

Authors: J. P. Crutchfield, C. J. Ellison, P. M. Riechers

Keywords: excess entropy, statistical complexity, projection operator, residual, resolvent, entropy rate, predictable information, bound information, ephemeral information

Abstract: We give exact formulae for a wide family of complexity measures that capture the organization of hidden nonlinear processes. The spectral decomposition of operator-valued functions leads to closed-form expressions involving the full eigenvalue spectrum of the mixed-state presentation of a process's γ -machine causal-state dynamic. Measures include correlation functions, power spectra, past-future mutual information, transient and synchronization informations, and many others. As a result, a direct and complete analysis of intrinsic computation is now available for the temporal organization of finitary hidden Markov models and nonlinear dynamical systems with generating partitions and for the spatial organization in one-dimensional systems, including spin systems, cellular automata, and complex materials via chaotic crystallography.

Distribution Statement: 3-Distribution authorized to U.S. Government Agencies and their contractors

Acknowledged Federal Support: Y

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published

Journal: Entropy

Publication Identifier Type:

Publication Identifier: 10.3390/e17074891

Volume: 17

Issue: 0

First Page #: 4891

Date Submitted: 8/26/17 12:00AM

Date Published:

Publication Location:

Article Title: Informational and Causal Architecture of Discrete-Time Renewal Processes

Authors: Sarah Marzen, James P. Crutchfield

Keywords: stationary renewal process, statistical complexity, predictable information, information anatomy, entropy rate

Abstract: Renewal processes are broadly used to model stochastic behavior consisting of isolated events separated by periods of quiescence, whose durations are specified by a given probability law. Here, we identify the minimal sufficient statistic for their prediction (the set of causal states), calculate the historical memory capacity required to store those states (statistical complexity), delineate what information is predictable (excess entropy), and decompose the entropy of a single measurement into that shared with the past, future, or both. The causal state equivalence relation defines a new subclass of renewal processes with a finite number of causal states despite having an unbounded interevent count distribution. We use these formulae to analyze the output of the parametrized Simple Nonunifilar Source, generated by a simple two-state hidden Markov model, but with an infinite-state γ -machine presentation. All in all, the results lay the groundwork for analyzing processes with infinite

Distribution Statement: 3-Distribution authorized to U.S. Government Agencies and their contractors

Acknowledged Federal Support: Y

RPPR Final Report as of 14-Jan-2021

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published

Journal: ACS Nano

Publication Identifier Type: DOI

Publication Identifier: 10.1021/nn502431c

Volume: 8

Issue: 5

First Page #: 0

Date Submitted:

Date Published:

Publication Location:

Article Title: The Ecology of Technology and Nanomotors

Authors:

Keywords: scaling laws, allometric scaling, evolution of technology

Abstract: Ecosystems are characterized by particular scaling laws describing, for example, the relationship between animal abundance and species body weight. It is hypothesized that technological systems follow similar scaling laws, where the abundance of a type of machine correlates with its size. Human progress continuously expands the range of accessible machine sizes, creating a technology trend toward vast numbers of microscopic machines. Current research related to nanomotors, such as the report by Kumar et al. in this issue of ACS Nano describing advances in controlling biomolecular motors, lays the scientific foundation for this trend.

Distribution Statement: 1-Approved for public release; distribution is unlimited.

Acknowledged Federal Support:

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published

Journal: Physics Today

Publication Identifier Type: DOI

Publication Identifier: 10.1063/PT.3.2490

Volume: 67

Issue: 8

First Page #: 0

Date Submitted:

Date Published:

Publication Location:

Article Title: Engineering Maxwell's demon

Authors:

Keywords: dissipation, information, measurement, control, efficiency

Abstract: A simple model illustrates the operating principles of an information engine, a mechanical device that mimics the behavior of Maxwell's demon by converting heat into information plus work.

Distribution Statement: 1-Approved for public release; distribution is unlimited.

Acknowledged Federal Support:

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published

Journal: PHYSICAL REVIEW E

Publication Identifier Type:

Publication Identifier:

Volume: 8.9E+001

Issue: 0

First Page #: 52140

Date Submitted:

Date Published:

Publication Location:

Article Title: Optimal Finite-time Erasure of a Classical Bit

Authors:

Keywords: information erasure, optimal control, minimal dissipation

Abstract: Information erasure inevitably leads to the generation of heat. Minimizing this dissipation will be crucial for developing small-scale information processing systems, but little is known about the optimal procedures required. We have obtained closed-form expressions for maximally efficient erasure cycles for deletion of a classical bit of information stored by the position of a particle diffusing in a double-well potential. We find that the extra heat generated beyond the Landauer bound is proportional to the square of the Hellinger distance between the initial and final states divided by the cycle duration, which quantifies how far out of equilibrium the system is driven. Finally, we demonstrate close agreement between the exact optimal cycle and the protocol found using a linear response framework.

Distribution Statement: 3-Distribution authorized to U.S. Government Agencies and their contractors

Acknowledged Federal Support:

RPPR Final Report as of 14-Jan-2021

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published

Journal: Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences

Publication Identifier Type:

Publication Identifier:

Volume: 4.71E+002 Issue: 0

First Page #: 1

Date Submitted:

Date Published:

Publication Location:

Article Title: Optimality, reduction and collective motion

Authors:

Keywords: collective behaviour, optimal control, maximum principle, symmetry reduction, explicit integrability, Poisson structure

Abstract: The planar self-steering particle model of agents in a collective gives rise to dynamics on the N-fold direct product of $SE(2)$, the rigid motion group in the plane. Assuming a connected, undirected graph of interaction between agents, we pose a family of symmetric optimal control problems with a coupling parameter capturing the strength of interactions. The Hamiltonian system associated with the necessary conditions for optimality is reducible to a Lie–Poisson dynamical system possessing interesting structure. In particular, the strong coupling limit reveals additional (hidden) symmetry, beyond the manifest one used in reduction: this enables explicit integration of the dynamics, and demonstrates the presence of a ‘master clock’ that governs all agents to steer identically. For finite coupling strength, we show that special solutions exist with steering controls proportional across the collective. These results suggest that optimality principles may provide a framework for understanding

Distribution Statement: 3-Distribution authorized to U.S. Government Agencies and their contractors
Acknowledged Federal Support:

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published

Journal: Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences

Publication Identifier Type:

Publication Identifier:

Volume: 4.71E+002 Issue: 0

First Page #: 1

Date Submitted:

Date Published:

Publication Location:

Article Title: Optimality, reduction and collective motion

Authors:

Keywords: collective behaviour, optimal control, maximum principle, symmetry reduction, explicit integrability, Poisson structure

Abstract: The planar self-steering particle model of agents in a collective gives rise to dynamics on the N-fold direct product of $SE(2)$, the rigid motion group in the plane. Assuming a connected, undirected graph of interaction between agents, we pose a family of symmetric optimal control problems with a coupling parameter capturing the strength of interactions. The Hamiltonian system associated with the necessary conditions for optimality is reducible to a Lie–Poisson dynamical system possessing interesting structure. In particular, the strong coupling limit reveals additional (hidden) symmetry, beyond the manifest one used in reduction: this enables explicit integration of the dynamics, and demonstrates the presence of a ‘master clock’ that governs all agents to steer identically. For finite coupling strength, we show that special solutions exist with steering controls proportional across the collective. These results suggest that optimality principles may provide a framework for understanding

Distribution Statement: 3-Distribution authorized to U.S. Government Agencies and their contractors
Acknowledged Federal Support:

RPPR Final Report as of 14-Jan-2021

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published

Journal: Nature Physics

Publication Identifier Type:

Publication Identifier:

Volume: 1.05E+002 Issue: 0

First Page #: 105

Date Submitted:

Date Published:

Publication Location:

Article Title: Diverse phenomena, common themes

Authors:

Keywords: nonequilibrium thermodynamics, fluctuation theorems

Abstract: Our framework for understanding non-equilibrium behaviour is yet to match the simplicity and power of equilibrium statistical physics. But recent theoretical and experimental advances reveal key principles that unify seemingly unrelated topics.

Distribution Statement: 3-Distribution authorized to U.S. Government Agencies and their contractors

Acknowledged Federal Support:

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published

Journal: PHYSICAL REVIEW E

Publication Identifier Type:

Publication Identifier:

Volume: 9.1E+001 Issue: 0

First Page #: 50106

Date Submitted:

Date Published:

Publication Location:

Article Title: Signatures of infinity: Nonergodicity and resource scaling in prediction, complexity, and learning

Authors:

Keywords: information divergence, excess entropy, hierarchy

Abstract: We introduce a simple analysis of the structural complexity of infinite-memory processes built from random samples of stationary, ergodic finite-memory component processes. Such processes are familiar from the well known multiarm Bandit problem. We contrast our analysis with computation-theoretic and statistical inference approaches to understanding their complexity. The result is an alternative view of the relationship between predictability, complexity, and learning that highlights the distinct ways in which informational and correlational divergences arise in complex ergodic and nonergodic processes. We draw out consequences for the resource divergences that delineate the structural hierarchy of ergodic processes and for processes that are themselves hierarchical.

Distribution Statement: 3-Distribution authorized to U.S. Government Agencies and their contractors

Acknowledged Federal Support:

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published

Journal: Journal of Statistical Physics

Publication Identifier Type:

Publication Identifier:

Volume: 0 Issue: 0

First Page #: 1

Date Submitted:

Date Published:

Publication Location:

Article Title: Computational Mechanics of Input-Output Processes: Structured transformations and the ϵ -transducer

Authors:

Keywords: Sequential machine, Communication channel, Finite-state transducer, Statistical complexity, Causal state, Minimality, Optimal prediction, Subshift endomorphism

Abstract: Computational mechanics quantifies structure in a stochastic process via its causal states, leading to the process's minimal, optimal predictor—the ϵ -machine. We extend computational mechanics to communication channels coupling two processes, obtaining an analogous optimal model—the epsilon-transducer—of the stochastic mapping between them. Here, we lay the foundation of a structural analysis of communication channels, treating joint processes and processes with input. The result is a principled structural analysis of mechanisms that support information flow between processes. It is the first in a series on the structural information theory of memoryful channels, channel composition, and allied conditional information measures.

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Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published

Journal: Current Opinion in Chemical Engineering

Publication Identifier Type:

Publication Identifier:

Volume: 7.0E+000 Issue: 0

First Page #: 47

Date Submitted:

Date Published:

Publication Location:

Article Title: Chaotic crystallography: how the physics of information reveals structural order in materials

Authors:

Keywords: crsytal structural, disorder, information, organization, structure, entropy

Abstract: We review recent progress in applying information-theoretic and computation-theoretic measures to describe material structure that transcends previous methods based on exact geometric symmetries. We discuss the necessary theoretical background for this new toolset and show how the new techniques detect and describe novel material properties. We discuss how the approach relates to well known crystallographic practice and examine how it provides novel interpretations of familiar structures. Throughout, we concentrate on disordered materials that, while important, have received less attention both theoretically and experimentally than those with either periodic or aperiodic order.

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Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published

Journal: Acta Crystallographica Section A Foundations and Advances

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Publication Identifier:

Volume: 7.1E+001 Issue: 0

First Page #: 423

Date Submitted:

Date Published:

Publication Location:

Article Title: Pairwise correlations in layered close-packed structures

Authors:

Keywords: X-ray diffraction; planar disorder; stacking fault; z-transformation; spectral decomposition; pair distribution function

Abstract: Given a description of the stacking statistics of layered close-packed structures in the form of a hidden Markov model, analytical expressions are developed for the pairwise correlation functions between the layers. These may be calculated analytically as explicit functions of model parameters or the expressions may be used as a fast, accurate and efficient way to obtain numerical values. Several examples are presented, finding agreement with previous work as well as deriving new relations.

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Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published

Journal: Frontiers of Computational Neuroscience

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Volume: 9.0E+000 Issue: 0

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Date Submitted:

Date Published:

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Article Title: Time resolution dependence of information measures for spiking neurons: scaling and universality

Authors:

Keywords: statistical complexity, excess entropy, entropy rate, renewal process, alternating renewal process, 102integrate and fire neuron, leaky integrate and fire neuron, quadratic integrate and fire neuron

Abstract: The mutual information between stimulus and spike-train response is commonly used to monitor neural coding efficiency, but neuronal computation broadly conceived requires more refined and targeted information measures of input-output joint processes. A first step toward that larger goal is to develop information measures for individual output processes, including information generation (entropy rate), stored information (statistical complexity), predictable information (excess entropy), and active information accumulation (bound information rate). We calculate these for spike trains generated by a variety of noise-driven integrate-and-fire neurons as a function of time resolution and for alternating renewal processes. We show that their time-resolution dependence reveals coarse-grained structural properties of interspike interval statistics; e.g., γ -entropy rates that diverge less quickly than the firing rate indicate interspike interval correlations. We also find evidence that

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Journal: Entropy

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Volume: 1.7E+001 Issue: 0

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Date Submitted:

Date Published:

Publication Location:

Article Title: Informational and Causal Architecture of Discrete-Time Renewal Processes

Authors:

Keywords: stationary renewal process; statistical complexity; predictable information; information anatomy; entropy rate

Abstract: Renewal processes are broadly used to model stochastic behavior consisting of isolated events separated by periods of quiescence, whose durations are specified by a given probability law. Here, we identify the minimal sufficient statistic for their prediction (the set of causal states), calculate the historical memory capacity required to store those states (statistical complexity), delineate what information is predictable (excess entropy), and decompose the entropy of a single measurement into that shared with the past, future, or both. The causal state equivalence relation defines a new subclass of renewal processes with a finite number of causal states despite having an unbounded interevent count distribution. We use the resulting formulae to analyze the output of the parametrized Simple Nonunifilar Source, generated by a simple two-state hidden Markov model, but with an infinite-state λ -machine presentation. All in all, the results lay the groundwork for analyzing more complex pro

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Journal: Physical Review E

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Publication Identifier: 10.1103/PhysRevE.92.042911

Volume: 92

Issue: 0

First Page #: 042911

Date Submitted: 8/29/17 12:00AM

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Publication Location:

Article Title: Universal energy diffusion in a quivering billiard

Authors: Jeffery Demers, Christopher Jarzynski

Keywords: billiard, hard sphere, Fermi-Ulam model, energy distribution

Abstract: We introduce and study a model of time-dependent billiard systems with billiard boundaries undergoing infinitesimal wiggling motions. The so-called quivering billiard is simple to simulate, straightforward to analyze, and is a faithful representation of time-dependent billiards in the limit of small boundary displacements. We assert that when a billiard's wall motion approaches the quivering motion, deterministic particle dynamics become inherently stochastic. Particle ensembles in a quivering billiard are shown to evolve to a universal energy distribution through an energy diffusion process, regardless of the billiard's shape or dimensionality, and as a consequence universally display Fermi acceleration. Our model resolves a known discrepancy between the one-dimensional Fermi-Ulam model and the simplified static wall approximation. We argue that a quivering billiard is the true fixed wall limit of the Fermi-Ulam model.

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Publication Identifier: 10.3390/e19080427

Volume: 19

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Date Submitted: 8/28/17 12:00AM

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Publication Location:

Article Title: Minimum and maximum entropy distributions for binary systems with known means and pairwise correlations

Authors: B. F. Albanna, C. Hillar, J. Sohl-Dickstein, and M. R. DeWeese

Keywords: information theory; minimum entropy; maximum entropy; statistical mechanics; Ising model; pairwise correlations; compressed sensing; neural networks

Abstract: Maximum entropy models are increasingly being used to describe the collective activity of neural populations with measured mean neural activities and pairwise correlations, but the full space of probability distributions consistent with these constraints has not been explored. We provide upper and lower bounds on the entropy for the minimum entropy distribution over arbitrarily large collections of binary units with any fixed set of mean values and pairwise correlations. We also construct specific low-entropy distributions for several relevant cases. Surprisingly, the minimum entropy solution has entropy scaling logarithmically with system size for any set of first- and second-order statistics consistent with arbitrarily large systems. We further demonstrate that some sets of these low-order statistics can only be realized by small systems. Our results show how only small amounts of randomness are needed to mimic low-order statistical properties of highly entropic distributions, ...

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Publication Identifier: 10.1103/PhysRevLett.116.190601

Volume: 116 Issue: 0

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Date Submitted: 8/26/17 12:00AM

Date Published:

Publication Location:

Article Title: Maxwell Demon Dynamics: Deterministic Chaos, the Szilard Map, and the Intelligence of Thermodynamic Systems

Authors: A. B. Boyd, J. P. Crutchfield

Keywords: deterministic chaos, Lyapunov characteristic exponents, Markov partition, Landauer's Principle, measurement, erasure, memory, entropy rate, mutual information, dissipated work, control theory

Abstract: We introduce a deterministic chaotic system—the Szilard Map—that encapsulates the measurement, control, and erasure protocol by which Maxwellian Demons extract work from a heat reservoir. Implementing the Demon's control function in a dynamical embodiment, our construction symmetrizes Demon and thermodynamic system, allowing one to explore their functionality and recover the fundamental trade-off between the thermodynamic costs of dissipation due to measurement and due to erasure. The map's degree of chaos—captured by the Kolmogorov-Sinai entropy—is the rate of energy extraction from the heat bath. Moreover, an engine's statistical complexity quantifies the minimum necessary system memory for it to function. In this way, dynamical instability in the control protocol plays an essential and constructive role in intelligent thermodynamic systems.

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Journal: New Journal of Physics

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Volume: 18 Issue: 0

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Date Submitted: 8/26/17 12:00AM

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Publication Location:

Article Title: Identifying Functional Thermodynamics in Autonomous Maxwellian Ratchets

Authors: A. B. Boyd, D. Mandal, J. P. Crutchfield

Keywords: Maxwell's Demon, Maxwell's refrigerator, detailed balance, entropy rate, Second Law of thermodynamics

Abstract: We introduce a family of Maxwellian Demons for which correlations among information bearing degrees of freedom can be calculated exactly and in compact analytical form. This allows one to precisely determine Demon functional thermodynamic operating regimes, when previous methods either misclassify or simply fail due to approximations they invoke. This reveals that these Demons are more functional than previous candidates. They too behave either as engines, lifting a mass against gravity by extracting energy from a single heat reservoir, or as Landauer erasers, consuming external work to remove information from a sequence of binary symbols by decreasing their individual uncertainty. Going beyond these, our Demon exhibits a new functionality that erases bits not by simply decreasing individual-symbol uncertainty, but by increasing inter-bit correlations (that is, by adding temporal order) while increasing single-symbol uncertainty. In all cases, but especially ...

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Publication Identifier: 1412.8520

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Date Submitted: 8/26/17 12:00AM

Date Published:

Publication Location:

Article Title: Understanding and Designing Complex Systems: Response to “A framework for optimal high-level descriptions in science and engineering—preliminary report”

Authors: J. P. Crutchfield, R. G. James, S. Marzen, D. P. Varn

Keywords: information theory, rate-distortion theory, computational mechanics, information bottleneck, macrostates, microstates, statistical physics, coarse-graining, dimension reduction, minimum description length

Abstract: We recount recent history behind building compact models of nonlinear, complex processes and identifying their relevant macroscopic patterns or “macrostates”. We give a synopsis of computational mechanics, predictive rate-distortion theory, and the role of information measures in monitoring model complexity and predictive performance. Computational mechanics provides a method to extract the optimal minimal predictive model for a given process. Rate-distortion theory provides methods for systematically approximating such models. We end by commenting on future prospects for developing a general framework that automatically discovers optimal compact models. As a response to the manuscript cited in the title above, this brief commentary corrects potentially misleading claims about its state space compression method and places it in a broader historical setting.

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Journal: Journal of Statistical Physics

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Volume: 163

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Date Submitted: 8/26/17 12:00AM

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Article Title: Predictive Rate-Distortion for Infinite-Order Markov Processes

Authors: S. Marzen, J. P. Crutchfield

Keywords: optimal causal filtering, computational mechanics, epsilon-machine, causal states, predictive rate-distortion, information bottleneck

Abstract: Predictive rate-distortion analysis suffers from the curse of dimensionality: clustering arbitrarily long pasts to retain information about arbitrarily long futures requires resources that typically grow exponentially with length. The challenge is compounded for infinite-order Markov processes, since conditioning on finite sequences cannot capture all of their past dependencies. Spectral arguments confirm a popular intuition: algorithms that cluster finite-length sequences fail dramatically when the underlying process has long-range temporal correlations and can fail even for processes generated by finite-memory hidden Markov models. We circumvent the curse of dimensionality in rate-distortion analysis of finite- and infinite-order processes by casting predictive rate-distortion objective functions in terms of the forward- and reverse-time causal states of computational mechanics. Examples demonstrate that the resulting algorithms yield substantial improvements.

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Journal: Physical Review E

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Publication Identifier: 10.1103/PhysRevE.93.042129

Volume: 93

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Date Submitted: 8/28/17 12:00AM

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Publication Location:

Article Title: Nonequilibrium work energy relation for non-Hamiltonian dynamics

Authors: Dibyendu Mandal, Michael R. DeWeese

Keywords: free energy, integral fluctuation theorem, dissipative system

Abstract: Recent years have witnessed major advances in our understanding of nonequilibrium processes. The Jarzynski equality, for example, provides a link between equilibrium free energy differences and finite-time nonequilibrium dynamics. We propose a generalization of this relation to non-Hamiltonian dynamics, relevant for active matter systems, continuous feedback, and computer simulation. Surprisingly, this relation allows us to calculate the free energy difference between the desired initial and final equilibrium states using arbitrary dynamics. As a practical matter, this dissociation between the dynamics and the initial and final states promises to facilitate a range of techniques for free energy estimation in a single universal expression.

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Date Submitted: 8/26/17 12:00AM

Date Published:

Publication Location:

Article Title: Memoryless Thermodynamics? A Reply

Authors: D. Mandal, A. B. Boyd, J. P. Crutchfield

Keywords: information ratchet, second law of thermodynamics, Shannon entropy rate

Abstract: We reply to arXiv:1508.00203 'Comment on "Identifying Functional Thermodynamics in Autonomous Maxwellian Ratchets"' (arXiv:1507.01537v2).

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Journal: Physical Review E

Publication Identifier Type: DOI

Publication Identifier: 10.1103/PhysRevE.92.032113

Volume: 92

Issue: 3

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Date Submitted: 8/29/16 12:00AM

Date Published: 9/1/15 7:00AM

Publication Location:

Article Title: Optimal protocols for slowly driven quantum systems

Authors: Patrick R. Zulkowski, Michael R. DeWeese

Keywords: information entropy

Abstract: The design of efficient quantum information processing will rely on optimal nonequilibrium transitions of driven quantum systems. Building on a recently developed geometric framework for computing optimal protocols for classical systems driven in finite time, we construct a general framework for optimizing the average information entropy for driven quantum systems. Geodesics on the parameter manifold endowed with a positive semidefinite metric correspond to protocols that minimize the average information entropy production in finite time. We use this framework to explicitly compute the optimal entropy production for a simple two-state quantum system coupled to a heat bath of bosonic oscillators, which has applications to quantum annealing.

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Volume: 92

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Date Submitted: 8/29/16 12:00AM

Date Published: 9/1/15 7:00AM

Publication Location:

Article Title: Optimal control of overdamped systems

Authors: Patrick R. Zulkowski, Michael R. DeWeese

Keywords: Riemannian geometry

Abstract: Nonequilibrium physics encompasses a broad range of natural and synthetic small-scale systems. Optimizing transitions of such systems will be crucial for the development of nanoscale technologies and may reveal the physical principles underlying biological processes at the molecular level. Recent work has demonstrated that when a thermodynamic system is driven away from equilibrium then the space of controllable parameters has a Riemannian geometry induced by a generalized inverse diffusion tensor. We derive a simple, compact expression for the inverse diffusion tensor that depends solely on equilibrium information for a broad class of potentials. We use this formula to compute the minimal dissipation for two model systems relevant to small-scale information processing and biological molecular motors. In the first model, we optimally erase a single classical bit of information modeled by an overdamped particle in a smooth double-well potential.

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Volume: 93

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Date Submitted: 8/29/16 12:00AM

Date Published: 2/1/16 8:00AM

Publication Location:

Article Title: Elusive present: Hidden past and future dependency and why we build models

Authors: Pooneh M. Ara, Ryan G. James, James P. Crutchfield

Keywords: Markov failure

Abstract: Modeling a temporal process as if it is Markovian assumes that the present encodes all of a process's history. When this occurs, the present captures all of the dependency between past and future. We recently showed that if one randomly samples in the space of structured processes, this is almost never the case. So, how does the Markov failure come about? That is, how do individual measurements fail to encode the past? and How many are needed to capture dependencies between the past and future? Here, we investigate how much information can be shared between the past and the future but not reflected in the present. We quantify this elusive information, give explicit calculational methods, and outline the consequences, the most important of which is that when the present hides past-future correlation or dependency we must move beyond sequence-based statistics and build state-based models.

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Volume: 116 Issue: 19

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Date Submitted: 8/29/16 12:00AM

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Publication Location:

Article Title: Maxwell Demon Dynamics: Deterministic Chaos, the Szilard Map, and the Intelligence of Thermodynamic Systems

Authors: Alexander B. Boyd, James P. Crutchfield

Keywords: Maxwellian demons

Abstract: We introduce a deterministic chaotic system—the Szilard map—that encapsulates the measurement, control, and erasure protocol by which Maxwellian demons extract work from a heat reservoir. Implementing the demon's control function in a dynamical embodiment, our construction symmetrizes the demon and the thermodynamic system, allowing one to explore their functionality and recover the fundamental trade-off between the thermodynamic costs of dissipation due to measurement and those due to erasure. The map's degree of chaos—captured by the Kolmogorov-Sinai entropy—is the rate of energy extraction from the heat bath. Moreover, an engine's statistical complexity quantifies the minimum necessary system memory for it to function. In this way, dynamical instability in the control protocol plays an essential and constructive role in intelligent thermodynamic systems.

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Date Submitted: 8/29/16 12:00AM

Date Published: 2/1/16 8:00AM

Publication Location:

Article Title: Identifying functional thermodynamics in autonomous Maxwellian ratchets

Authors: Alexander B Boyd, Dibyendu Mandal, James P Crutchfield

Keywords: Second Law of thermodynamics, Kolmogorov-Sinai entropy

Abstract: We introduce a family of Maxwellian Demons for which correlations among information bearing degrees of freedom can be calculated exactly and in compact analytical form. This allows one to precisely determine Demon functional thermodynamic operating regimes, when previous methods either misclassify or simply fail due to approximations they invoke. This reveals that these Demons are more functional than previous candidates. They too behave either as engines, lifting a mass against gravity by extracting energy from a single heat reservoir, or as Landauer erasers, consuming external work to remove information from a sequence of binary symbols by decreasing their individual uncertainty.

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Volume: 380

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Date Submitted: 8/29/16 12:00AM

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Publication Location:

Article Title: Exact complexity: The spectral decomposition of intrinsic computation

Authors: James P. Crutchfield, Christopher J. Ellison, Paul M. Riechers

Keywords: Excess entropy, Statistical complexity, Projection operator, Resolvent, Entropy rate, Predictable information

Abstract: We give exact formulae for a wide family of complexity measures that capture the organization of hidden nonlinear processes. The spectral decomposition of operator-valued functions leads to closed-form expressions involving the full eigenvalue spectrum of the mixed-state presentation of a process's ϵ -machine causal-state dynamic. Measures include correlation functions, power spectra, past-future mutual information, transient and synchronization informations, and many others. As a result, a direct and complete analysis of intrinsic computation is now available for the temporal organization of finitary hidden Markov models and nonlinear dynamical systems with generating partitions and for the spatial organization in one-dimensional systems, including spin systems, cellular automata, and complex materials via chaotic crystallography.

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Journal: Journal of Statistical Physics

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Volume: 163

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Date Submitted: 8/29/16 12:00AM

Date Published: 5/1/16 7:00AM

Publication Location:

Article Title: Predictive Rate-Distortion for Infinite-Order Markov Processes

Authors: Sarah E. Marzen, James P. Crutchfield

Keywords: Optimal causal filtering, Computational mechanics, Epsilon-machine, Causal states, Predictive rate-distortion, Information bottleneck

Abstract: Predictive rate-distortion analysis suffers from the curse of dimensionality: clustering arbitrarily long pasts to retain information about arbitrarily long futures requires resources that typically grow exponentially with length. The challenge is compounded for infinite-order Markov processes, since conditioning on finite sequences cannot capture all of their past dependencies. Spectral arguments confirm a popular intuition: algorithms that cluster finite-length sequences fail dramatically when the underlying process has long-range temporal correlations and can fail even for processes generated by finite-memory hidden Markov models. We circumvent the curse of dimensionality in rate-distortion analysis of finite- and infinite-order processes by casting predictive rate-distortion objective functions in terms of the forward- and reverse-time causal states of computational mechanics. Examples demonstrate that the resulting algorithms yield substantial improvements.

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Date Submitted: 8/29/16 12:00AM

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Publication Location:

Article Title: Information Flows? A Critique of Transfer Entropies

Authors: Ryan G. James, Nix Barnett, James P. Crutchfield

Keywords: transfer entropy

Abstract: A central task in analyzing complex dynamics is to determine the loci of information storage and the communication topology of information flows within a system. Over the last decade and a half, diagnostics for the latter have come to be dominated by the transfer entropy. Via straightforward examples, we show that it and a derivative quantity, the causation entropy, do not, in fact, quantify the flow of information. At one and the same time they can overestimate flow or underestimate influence. We isolate why this is the case and propose several avenues to alternate measures for information flow. We also address an auxiliary consequence: The proliferation of networks as a now-common theoretical model for large-scale systems, in concert with the use of transferlike entropies, has shoehorned dyadic relationships into our structural interpretation of the organization and behavior of complex systems. This interpretation thus fails to include the effects of polyadic dependencies.

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Volume: 380 Issue: 17

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Publication Location:

Article Title: Statistical signatures of structural organization: The case of long memory in renewal processes

Authors: Sarah E. Marzen, James P. Crutchfield

Keywords: Fractal renewal process, Statistical complexity, Excess entropy, Power-law scaling, 1/f noise, Zipf's law

Abstract: Identifying and quantifying memory are often critical steps in developing a mechanistic understanding of stochastic processes. These are particularly challenging and necessary when exploring processes that exhibit long-range correlations. The most common signatures employed rely on second-order temporal statistics and lead, for example, to identifying long memory in processes with power-law autocorrelation function and Hurst exponent greater than 1/2. However, most stochastic processes hide their memory in higher-order temporal correlations. Information measures—specifically, divergences in the mutual information between a process' past and future (excess entropy) and minimal predictive memory stored in a process' causal states (statistical complexity)—provide a different way to identify long memory in processes with higher-order temporal correlations.

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Journal: Physical Review A
Publication Identifier Type: DOI **Publication Identifier:** 10.1103/PhysRevA.93.052317
Volume: 93 **Issue:** 5 **First Page #:**
Date Submitted: 8/29/16 12:00AM **Date Published:** 5/1/16 7:00AM
Publication Location:

Article Title: Minimized state complexity of quantum-encoded cryptic processes

Authors: Paul M. Riechers, John R. Mahoney, Cina Aghamohammadi, James P. Crutchfield

Keywords: state complexity

Abstract: The predictive information required for proper trajectory sampling of a stochastic process can be more efficiently transmitted via a quantum channel than a classical one. This recent discovery allows quantum information processing to drastically reduce the memory necessary to simulate complex classical stochastic processes. It also points to a new perspective on the intrinsic complexity that nature must employ in generating the processes we observe. The quantum advantage increases with codeword length: the length of process sequences used in constructing the quantum communication scheme. In analogy with the classical complexity measure, statistical complexity, we use this reduced communication cost as an entropic measure of state complexity in the quantum representation. Previously difficult to compute, the quantum advantage is expressed here in closed form using spectral decomposition.

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Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences
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Volume: 374 **Issue:** 2063 **First Page #:** 20150067
Date Submitted: 8/29/16 12:00AM **Date Published:** 2/1/16 12:00AM
Publication Location:

Article Title: What did Erwin mean? The physics of information from the materials genomics of aperiodic crystals and water to molecular information catalysts and life

Authors: D. P. Varn, J. P. Crutchfield

Keywords: entropy, randomness, disorder, structure, mutual information, Maxwell's Demon

Abstract: Erwin Schrödinger famously and presciently ascribed the vehicle transmitting the hereditary information underlying life to an 'aperiodic crystal'. We compare and contrast this, only later discovered to be stored in the linear biomolecule DNA, with the information-bearing, layered quasi-one-dimensional materials investigated by the emerging field of chaotic crystallography. Despite differences in functionality, the same information measures capture structure and novelty in both, suggesting an intimate coherence between the information character of biotic and abiotic matter—a broadly applicable physics of information. We review layered solids and consider three examples of how information- and computation-theoretic techniques are being applied to understand their structure.

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Volume: 6

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First Page #: 20495

Date Submitted: 8/29/16 12:00AM

Date Published: 2/1/16 12:00AM

Publication Location:

Article Title: Occam's Quantum Strop: Synchronizing and Compressing Classical Cryptic Processes via a Quantum Channel

Authors: John R. Mahoney, Cina Aghamohammadi, James P. Crutchfield

Keywords: quantum state-indistinguishability

Abstract: A stochastic process' statistical complexity stands out as a fundamental property: the minimum information required to synchronize one process generator to another. How much information is required, though, when synchronizing over a quantum channel? Recent work demonstrated that representing causal similarity as quantum state-indistinguishability provides a quantum advantage. We generalize this to synchronization and offer a sequence of constructions that exploit extended causal structures, finding substantial increase of the quantum advantage. We demonstrate that maximum compression is determined by the process' cryptic order—a classical, topological property closely allied to Markov order, itself a measure of historical dependence. We introduce an efficient algorithm that computes the quantum advantage and close noting that the advantage comes at a cost—one trades off prediction for generation complexity.

Distribution Statement: 3-Distribution authorized to U.S. Government Agencies and their contractors

Acknowledged Federal Support: Y

Publication Type: Journal Article

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Publication Identifier: 10.1103/PhysRevE.92.042911

Volume: 92

Issue: 4

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Date Submitted: 8/29/16 12:00AM

Date Published: 10/1/15 7:00AM

Publication Location:

Article Title: Universal energy diffusion in a quivering billiard

Authors: Jeffery Demers, Christopher Jarzynski

Keywords: universal energy distribution, energy diffusion

Abstract: We introduce and study a model of time-dependent billiard systems with billiard boundaries undergoing infinitesimal wiggling motions. The so-called quivering billiard is simple to simulate, straightforward to analyze, and is a faithful representation of time-dependent billiards in the limit of small boundary displacements. We assert that when a billiard's wall motion approaches the quivering motion, deterministic particle dynamics become inherently stochastic. Particle ensembles in a quivering billiard are shown to evolve to a universal energy distribution through an energy diffusion process, regardless of the billiard's shape or dimensionality, and as a consequence universally display Fermi acceleration. Our model resolves a known discrepancy between the one-dimensional Fermi-Ulam model and the simplified static wall approximation. We argue that the quivering limit is the true fixed wall limit of the Fermi-Ulam model.

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Date Submitted: 8/29/16 12:00AM

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Publication Location:

Article Title: Nonequilibrium work energy relation for non-Hamiltonian dynamics

Authors: Dibyendu Mandal, Michael R. DeWeese

Keywords: Nonequilibrium work energy

Abstract: Recent years have witnessed major advances in our understanding of nonequilibrium processes. The Jarzynski equality, for example, provides a link between equilibrium free energy differences and finite-time nonequilibrium dynamics. We propose a generalization of this relation to non-Hamiltonian dynamics, relevant for active matter systems, continuous feedback, and computer simulation. Surprisingly, this relation allows us to calculate the free energy difference between the desired initial and final equilibrium states using arbitrary dynamics. As a practical matter, this dissociation between the dynamics and the initial and final states promises to facilitate a range of techniques for free energy estimation in a single universal expression.

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Journal: Journal of Statistical Mechanics: Theory and Experiment

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Volume: 2016

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Date Submitted: 8/29/16 12:00AM

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Publication Location:

Article Title: Analysis of slow transitions between nonequilibrium steady states

Authors: Dibyendu Mandal, Christopher Jarzynski

Keywords: fluctuation phenomena, stationary states, stochastic processes, correlation functions

Abstract: Transitions between nonequilibrium steady states obey a generalized Clausius inequality, which becomes an equality in the quasistatic limit. For slow but finite transitions, we show that the behavior of the system is described by a response matrix whose elements are given by a far-from-equilibrium Green-Kubo formula, involving the decay of correlations evaluated in the nonequilibrium steady state. This result leads to a fluctuation-dissipation relation between the mean and variance of the nonadiabatic entropy production, σ_{na} . Furthermore, our results extend—to nonequilibrium steady states—the thermodynamic metric structure introduced by Sivak and Crooks for analyzing minimal-dissipation protocols for transitions between equilibrium states.

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Journal: Langmuir

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Volume: 32

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Date Submitted: 8/29/16 12:00AM

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Publication Location:

Article Title: Velocity Fluctuations in Kinesin-1 Gliding Motility Assays Originate in Motor Attachment Geometry Variations

Authors: Henri Palacci, Ofer Idan, Megan J. Armstrong, Ashutosh Agarwal, Takahiro Nitta, Henry Hess

Keywords: motor protein

Abstract: Motor proteins such as myosin and kinesin play a major role in cellular cargo transport, muscle contraction, cell division, and engineered nanodevices. Quantifying the collective behavior of coupled motors is critical to our understanding of these systems. An excellent model system is the gliding motility assay, where hundreds of surface-adhered motors propel one cytoskeletal filament such as an actin filament or a microtubule. The filament motion can be observed using fluorescence microscopy, revealing fluctuations in gliding velocity. These velocity fluctuations have been previously quantified by a motional diffusion coefficient, which Sekimoto and Tawada explained as arising from the addition and removal of motors from the linear array of motors propelling the filament as it advances, assuming that different motors are not equally efficient in their force generation.

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Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published

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Publication Identifier: 10.1039/C5SM02042E

Volume: 12

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Date Submitted: 8/29/16 12:00AM

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Publication Location:

Article Title: Cytoskeletal motor-driven active self-assembly in in vitro systems

Authors: A. T. Lam, V. VanDelinder, A. M. R. Kabir, H. Hess, G. D. Bachand, A. Kakugo

Keywords: passive self-assembly

Abstract: Molecular motor-driven self-assembly has been an active area of soft matter research for the past decade. Because molecular motors transform chemical energy into mechanical work, systems which employ molecular motors to drive self-assembly processes are able to overcome kinetic and thermodynamic limits on assembly time, size, complexity, and structure. Here, we review the progress in elucidating and demonstrating the rules and capabilities of motor-driven active self-assembly. We focus on the types of structures created and the degree of control realized over these structures, and discuss the next steps necessary to achieve the full potential of this assembly mode which complements robotic manipulation and passive self-assembly.

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Volume: 6

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Date Submitted: 8/29/16 12:00AM

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Publication Location:

Article Title: Mimicking Nonequilibrium Steady States with Time-Periodic Driving

Authors: O. Raz, Y. Subasi, C. Jarzynski

Keywords: Statistical Physics

Abstract: Under static conditions, a system satisfying detailed balance generically relaxes to an equilibrium state in which there are no currents. To generate persistent currents, either detailed balance must be broken or the system must be driven in a time-dependent manner. A stationary system that violates detailed balance evolves to a nonequilibrium steady state (NESS) characterized by fixed currents. Conversely, a system that satisfies instantaneous detailed balance but is driven by the time-periodic variation of external parameters—also known as a stochastic pump (SP)—reaches a periodic state with nonvanishing currents. In both cases, these currents are maintained at the cost of entropy production. Are these two paradigmatic scenarios effectively equivalent? For discrete-state systems, we establish a mapping between nonequilibrium stationary states and stochastic pumps.

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Date Submitted: 8/29/16 12:00AM

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Publication Location:

Article Title: Leveraging information storage to select forecast-optimal parameters for delay-coordinate reconstructions

Authors: Joshua Garland, Ryan G. James, Elizabeth Bradley

Keywords: reconstruction-based forecast models

Abstract: Delay-coordinate reconstruction is a proven modeling strategy for building effective forecasts of nonlinear time series. The first step in this process is the estimation of good values for two parameters, the time delay and the embedding dimension. Many heuristics and strategies have been proposed in the literature for estimating these values. Few, if any, of these methods were developed with forecasting in mind, however, and their results are not optimal for that purpose. Even so, these heuristics—intended for other applications—are routinely used when building delay coordinate reconstruction-based forecast models. In this paper, we propose an alternate strategy for choosing optimal parameter values for forecast methods that are based on delay-coordinate reconstructions. The basic calculation involves maximizing the shared information between each delay vector and the future state of the system.

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Date Submitted: 8/26/17 12:00AM

Date Published: 8/30/16 9:52AM

Publication Location:

Article Title: Correlation-powered Information Engines and the Thermodynamics of Self-Correction

Authors: A. B. Boyd, D. Mandal, and J. P. Crutchfield

Keywords: Maxwell's Demon, Maxwell's refrigerator, detailed balance, entropy rate, Second Law of Thermodynamics

Abstract: Information engines can use structured environments as a resource to generate work by randomizing ordered inputs and leveraging the increased Shannon entropy to transfer energy from a thermal reservoir to a work reservoir. We give a broadly applicable expression for the work production of an information engine, generally modeled as a memoryful channel that communicates inputs to outputs as it interacts with an evolving environment. The expression establishes that an information engine must have more than one memory state in order to leverage input environment correlations. To emphasize this functioning, we designed an information engine powered solely by temporal correlations and not by statistical biases, as employed by previous engines. Key to this is the engine's ability to synchronize—the engine automatically returns to a desired dynamical phase when thrown into an unwanted, dissipative phase by corruptions in the input—that is, by unanticipated environmental fluctuations. ...

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Journal: Physics Letters A

Publication Identifier Type: DOI

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Volume: 381

Issue: 14

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Date Submitted: 8/26/17 12:00AM

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Publication Location:

Article Title: The Ambiguity of Simplicity in Quantum and Classical Simulation

Authors: C. Aghamohammadi, J. R. Mahoney, and J. P. Crutchfield

Keywords: stochastic process, hidden Markov model, ?-machine, causal states, mutual information

Abstract: A system's perceived simplicity depends on whether it is represented classically or quantumly. This is not so surprising, as classical and quantum physics are descriptive frameworks built on different assumptions that capture, emphasize, and express different properties and mechanisms. What is surprising is that, as we demonstrate, simplicity is ambiguous: the relative simplicity between two systems can change sign when moving between classical and quantum descriptions. Here, we associate simplicity with small model-memory. We see that the notions of absolute physical simplicity at best form a partial, not a total, order. This suggests that appeals to principles of physical simplicity, via Ockham's Razor or to the "elegance" of competing theories, may be fundamentally subjective. Recent rapid progress in quantum computation and quantum simulation suggest that the ambiguity of simplicity will strongly impact statistical inference and, in particular, model selection.

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Date Submitted: 8/26/17 12:00AM

Date Published: 8/17/16 2:57AM

Publication Location:

Article Title: Anatomy of a Spin: The Information-Theoretic Structure of Classical Spin Systems

Authors: V. S. Vijayaraghavan, R. G. James, and J. P. Crutchfield

Keywords: Ising spin model, thermodynamic entropy density, dual total correlation, entropy rate, elusive information, enigmatic information, predictable information rate, complex system

Abstract: Collective organization in matter plays a significant role in its expressed physical properties. Typically, it is detected via an order parameter, appropriately defined for each given system's observed emergent patterns. Recent developments in information theory, however, suggest quantifying collective organization in a system- and phenomenon-agnostic way: decomposing the system's thermodynamic entropy density into a localized entropy, that is solely contained in the dynamics at a single location, and a bound entropy, that is stored in space as domains, clusters, excitations, or other emergent structures. As a concrete demonstration, we compute this decomposition and related quantities explicitly for the nearest-neighbor Ising model on the 1D chain, on the Bethe lattice with coordination number $k = 3$, and on the 2D square lattice, illustrating its generality and the functional insights it gives near and away from phase transitions. In particular, we consider ...

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Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published

Journal: 55th IEEE Conference on Decision and Control

Publication Identifier Type: DOI

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Volume: 55

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Date Submitted: 8/30/17 12:00AM

Date Published: 12/15/16 5:06AM

Publication Location:

Article Title: Optimal Control of a Stochastic Oscillator in Non-equilibrium Thermodynamics

Authors: Y. Huang and P. S. Krishnaprasad

Keywords: Non-equilibrium thermodynamics, Optimal control, Maximum Principle, Collective behaviors

Abstract: A stochastic oscillator can be used as a model of nano-scale heat engine, whose stiffness of potential well and the inverse of heat bath temperature are control variables. The non-equilibrium dissipation in the space of its control variables has an inverse diffusion tensor and the control space is hyperbolic. To improve efficiency of a heat engine, it is necessary to minimize its dissipation, while the extracted work is prescribed. A stochastic oscillator may also be used in the analysis of the dynamics of a kinesin head. Due to the relation between the Lie group $SL(2, \mathbb{R})$ and hyperbolic space, the process of changing stochastic oscillator's control variables can be described as a left-invariant and non-holonomic dynamics in $SL(2, \mathbb{R})$. Further, the collective behaviors of N kinesin heads will be analyzed as N -folded direct product of $SL(2, \mathbb{R})$ in later half of this paper.

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Volume: 55

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Date Submitted: 8/30/17 12:00AM

Date Published: 12/15/16 4:09AM

Publication Location:

Article Title: Steering for Beacon Pursuit under Limited Sensing

Authors: U. Halder, B. Schlotfeldt, P. S. Krishnaprasad

Keywords: Beacon Pursuit, Collective Motion, Kepler Problem, Field-Of-View Constraint

Abstract: The focus of this paper is twofold. First, we investigate the behavior of two self-steering agents (particles) in a specific instance of pursuit where one agent uses a constant bearing strategy. The pursued agent is controlled independently. The interesting dynamic properties on an invariant manifold, emerging from analysis of this dyadic interaction, display a certain similarity to the two-body Kepler problem. Secondly, the results of this analysis are brought to bear on a practical problem of tracking a stationary beacon using a sensor with limited field of view (FOV). An effective solution to this problem is demonstrated in a laboratory implementation using a Kinect vision sensor mounted on a robot. Essential to this solution is the augmentation of the feedback law suggested by the first part with an odometry-driven estimator when the beacon falls outside of the FOV.

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Volume: 55

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Date Submitted: 8/30/17 12:00AM

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Publication Location:

Article Title: Motion camouflage in the presence of sensory noise and delay

Authors: V. Raju, P. S. Krishnaprasad

Keywords: two agent planar pursuit problem

Abstract: In this work, we discuss the feasibility of motion camouflage in the two agent planar pursuit problem in which the pursuer implements a feedback strategy employing delayed sensory information subject to noise, whose variance is inversely proportional to the delay. This variance-delay modeling assumption is intended to capture the tradeoff between the speed of computation and accuracy of information available to the pursuer. However, in this paper, we limit ourselves to fixed variance and a range of delays.

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Journal: Royal Society Proceedings A

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Volume: 472

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First Page #:

Date Submitted: 8/30/17 12:00AM

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Publication Location:

Article Title: Symmetry and Reduction in Collectives: Low-Dimensional Cyclic Pursuit

Authors: K. S. Galloway, E. W. Justh, P. S. Krishnaprasad

Keywords: ursuit strategy, cyclic pursuit, constant bearing, motion camouflage, steering law, symmetry group, shape dynamics, invariant manifold, relative equilibria, reduction, geometric methods

Abstract: We investigate low-dimensional examples of cyclic pursuit in a collective, wherein each agent employs a constant bearing (CB) steering law relative to exactly one other agent. For the case of three agents in the plane, we characterize relative equilibria and pure shape equilibria of associated closed loop dynamics. Re-scaling time yields a reduction of phase space to two dimensions and effective tools for stability analysis. Study of bifurcation of a family of collinear equilibria dependent on a single CB control parameter reveals the presence of a rich collection of trajectories that are periodic in shape and undergo precession in physical space. For collectives in three dimensions (3D), with an appropriate notion of CB pursuit strategy and corresponding steering law, the two-agent case proves to be explicitly integrable. These results suggest control schemes for small teams of mobile robotic agents engaged in area coverage tasks such as search-and-rescue, and raise interesting possi

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Volume: 473

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Date Submitted: 8/30/17 12:00AM

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Publication Location:

Article Title: Geometric Decompositions of Collective Motion

Authors: M. Mischiati, P. S. Krishnaprasad

Keywords: collective motion, ensemble properties, n-body problem, energy decomposition, fiber bundles, connections

Abstract: Collective motion in nature is a captivating phenomenon. Revealing the underlying mechanisms, which are of biological and theoretical interest, will require empirical data, modeling, and analysis techniques. Here we contribute a geometric viewpoint, yielding a novel method of analyzing movement. Snapshots of collective motion are portrayed as tangent vectors on configuration space, with length determined by the total kinetic energy. Using the geometry of fiber bundles and connections, this portrait is split into orthogonal components each tangential to a lower dimensional manifold derived from configuration space. The resulting decomposition, when interleaved with classical shape space construction, is categorized into a family of kinematic modes - including rigid translations, rigid rotations, inertia tensor transformations, expansions and compressions.

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Journal: Nature Nanotechnology
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Volume: **Issue:** **First Page #:**
Date Submitted: 8/29/16 12:00AM **Date Published:** 7/7/16 8:20PM
Publication Location:

Article Title: Adaptive non-equilibrium nanosystems with reversibly-bound molecular building blocks

Authors: 18. A. T. Lam and H. Hess

Keywords: microtubules, biomolecular motors

Abstract: Engineering molecular-scale systems that dynamically self-assemble and disassemble would allow us to create materials which mimic the way in which biological systems achieve self-healing and adaptation. However, this dynamic interplay of localized component recruitment and release has been difficult to achieve in artificial molecular-scale systems, which are often designed to have long-lasting, stable bonds. Here, we report the experimental realization of a molecular system that dynamically assembles and disassembles its building blocks while retaining functionality. In our system, filaments (microtubules) recruit biomolecular motors (kinesins) to a surface engineered to allow for the reversible binding of the kinesin motors. These recruited motors work to propel microtubules along the surface.

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Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: Physical Review E
Publication Identifier Type: DOI **Publication Identifier:** 10.1103/PhysRevE.92.060102
Volume: 92 **Issue:** 6 **First Page #:** 060102-1
Date Submitted: 8/29/16 12:00AM **Date Published:** 12/1/15 8:00AM
Publication Location:

Article Title: Optimal control in nonequilibrium systems: Dynamic Riemannian geometry of the Ising model

Authors: Grant M. Rotskoff, Gavin E. Crooks

Keywords: Riemannian metric, two-dimensional Ising model

Abstract: A general understanding of optimal control in nonequilibrium systems would illuminate the operational principles of biological and artificial nanoscale machines. Recent work has shown that a system driven out of equilibrium by a linear response protocol is endowed with a Riemannian metric related to generalized susceptibilities, and that geodesics on this manifold are the nonequilibrium control protocols with the lowest achievable dissipation. While this elegant mathematical framework has inspired numerous studies of exactly solvable systems, no description of the thermodynamic geometry yet exists when the metric cannot be derived analytically. Herein, we numerically construct the dynamic metric of the two-dimensional Ising model in order to study optimal protocols for reversing the net magnetization.

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Date Submitted: 8/28/17 12:00AM

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Publication Location:

Article Title: Thermodynamic geometry of minimum-dissipation driven barrier crossing

Authors: D. Sivak, G. E. Crooks

Keywords: barrier crossing, entropy, minimum dissipation, optimization

Abstract: We explore the thermodynamic geometry of a simple system that models the bistable dynamics of nucleic acid hairpins in single molecule force-extension experiments. Near equilibrium, optimal (minimum-dissipation) driving protocols are governed by a generalized linear response friction coefficient. Our analysis demonstrates that the friction coefficient of the driving protocols is sharply peaked at the interface between metastable regions, which leads to minimum-dissipation protocols that drive rapidly within a metastable basin, but then linger longest at the interface, giving thermal fluctuations maximal time to kick the system over the barrier. Intuitively, the same principle applies generically in free energy estimation (both in steered molecular dynamics simulations and in single-molecule experiments), provides a design principle for the construction of thermodynamically efficient coupling between stochastic objects, and makes a prediction regarding the construction of evolved ...

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Publication Location:

Article Title: Geometric approach to optimal nonequilibrium control: Minimizing dissipation in nanomagnetic spin systems

Authors: G. M. Rotskoff, G. E. Crooks, E. Vanden-Eijnden

Keywords: optimization, nonequilibrium, nanomagnetic, spintronics, minimum dissipation

Abstract: Optimal control of nanomagnets has become an urgent problem for the field of spintronics as technological tools approach thermodynamically determined limits of efficiency. In complex, fluctuating systems, such as nanomagnetic bits, finding optimal protocols is challenging, requiring detailed information about the dynamical fluctuations of the controlled system. We provide a physically transparent derivation of a metric tensor for which the length of a protocol is proportional to its dissipation. This perspective simplifies nonequilibrium optimization problems by recasting them in a geometric language. We then describe a numerical method, an instance of geometric minimum action methods, that enables computation of geodesics even when the number of control parameters is large. We apply these methods to two models of nanomagnetic bits: a LandauLifshitz-Gilbert description of a single magnetic spin controlled by two orthogonal magnetic fields, and a two-dimensional Ising model in which ...

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Publication Identifier Type: DOI **Publication Identifier:** 10.1103/PhysRevE.95.051301
Volume: 95 **Issue:** 5 **First Page #:** 051301-1
Date Submitted: 8/26/17 12:00AM **Date Published:** 5/1/17 7:00AM
Publication Location:

Article Title: Nearly maximally predictive features and their dimensions

Authors: Sarah E. Marzen, James P. Crutchfield

Keywords: hidden Markov models, entropy rate, dimension, resource-prediction trade-off, mixed-state simplex

Abstract: Scientific explanation often requires inferring maximally predictive features from a given data set. Unfortunately, the collection of minimal maximally predictive features for most stochastic processes is uncountably infinite. In such cases, one compromises and instead seeks nearly maximally predictive features. Here, we derive upper bounds on the rates at which the number and the coding cost of nearly maximally predictive features scale with desired predictive power. The rates are determined by the fractal dimensions of a process' mixed-state distribution. These results, in turn, show how widely used finite-order Markov models can fail as predictors and that mixed-state predictive features can offer a substantial improvement.

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Journal: Physical Review E
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Volume: 95 **Issue:** 6 **First Page #:** 060102-1
Date Submitted: 8/26/17 12:00AM **Date Published:** 6/1/17 7:00AM
Publication Location:

Article Title: Information trimming: Sufficient statistics, mutual information, and predictability from effective channel states

Authors: Ryan G. James, John R. Mahoney, James P. Crutchfield

Keywords: information theory, sufficient statistics, mutual information, dimensionality reduction, stochastic process, ?-machine, causal states, transmission rate

Abstract: One of the most basic characterizations of the relationship between two random variables, X and Y , is the value of their mutual information. Unfortunately, calculating it analytically and estimating it empirically are often stymied by the extremely large dimension of the variables. One might hope to replace such a high-dimensional variable by a smaller one that preserves its relationship with the other. It is well known that either X (or Y) can be replaced by its minimal sufficient statistic about Y (or X) while preserving the mutual information. While intuitively reasonable, it is not obvious or straightforward that both variables can be replaced simultaneously. We demonstrate that this is in fact possible: the information X 's minimal sufficient statistic preserves about Y is exactly the information that Y 's minimal sufficient statistic preserves about X . We call this procedure information trimming. As an important corollary, we consider ...

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Journal: Physical Review E
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Volume: 95 **Issue:** 6 **First Page #:** 062139-1
Date Submitted: 8/26/17 12:00AM **Date Published:** 6/1/17 7:00AM
Publication Location:

Article Title: Thermodynamics of random number generation

Authors: Cina Aghamohammadi, James P. Crutchfield

Keywords: entropy rate, nonequilibrium steady state, Maxwell's Demon, Second Law of Thermodynamics

Abstract: We analyze the thermodynamic costs of the three main approaches to generating random numbers via the recently introduced Information Processing Second Law. Given access to a specified source of randomness, a random number generator (RNG) produces samples from a desired target probability distribution. This differs from pseudorandom number generators (PRNGs) that use wholly deterministic algorithms and from true random number generators (TRNGs) in which the randomness source is a physical system. For each class, we analyze the thermodynamics of generators based on algorithms implemented as finite-state machines, as these allow for direct bounds on the required physical resources. This establishes bounds on heat dissipation and work consumption during the operation of three main classes of RNG algorithms—including those of von Neumann, Knuth, and Yao and Roche and Hoshi—and for PRNG methods. We introduce a general TRNG and determine its thermodynamic costs exactly for arbitrary ...

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Journal: Physical Review Letters
Publication Identifier Type: DOI **Publication Identifier:** 10.1103/PhysRevLett.118.220602
Volume: 118 **Issue:** 22 **First Page #:** 220602-1
Date Submitted: 8/26/17 12:00AM **Date Published:** 6/1/17 7:00AM
Publication Location:

Article Title: Transient Dissipation and Structural Costs of Physical Information Transduction

Authors: Alexander B. Boyd, Dibyendu Mandal, Paul M. Riechers, James P. Crutchfield

Keywords: transducer, intrinsic computation, Information-Processing Second Law of Thermodynamic

Abstract: A central result that arose in applying information theory to the stochastic thermodynamics of nonlinear dynamical systems is the information-processing second law (IPSL): the physical entropy of the Universe can decrease if compensated by the Shannon-Kolmogorov-Sinai entropy change of appropriate information-carrying degrees of freedom. In particular, the asymptotic-rate IPSL precisely delineates the thermodynamic functioning of autonomous Maxwellian demons and information engines. How do these systems begin to function as engines, Landauer erasers, and error correctors? We identify a minimal, and thus inescapable, transient dissipation of physical information processing, which is not captured by asymptotic rates, but is critical to adaptive thermodynamic processes such as those found in biological systems. A component of transient dissipation, we also identify an implementation-dependent cost that varies from one physical substrate to another for the same information processing ...

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Journal: Journal of Statistical Physics

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Volume: 168

Issue: 1

First Page #: 109

Date Submitted: 8/26/17 12:00AM

Date Published: 4/1/17 7:00AM

Publication Location:

Article Title: Informational and Causal Architecture of Continuous-time Renewal Processes

Authors: Sarah Marzen, James P. Crutchfield

Keywords: renewal process, entropy rate, excess entropy, statistical complexity, information anatomy, hidden semi-Markov models

Abstract: We introduce the minimal maximally predictive models (?-machines) of processes generated by certain hidden semi-Markov models. Their causal states are either discrete, mixed, or continuous random variables and causal-state transitions are described by partial differential equations. As an application, we present a complete analysis of the ?-machines of continuous-time renewal processes. This leads to closed-form expressions for their entropy rate, statistical complexity, excess entropy, and differential information anatomy rates.

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Journal: Journal of Statistical Physics

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Date Submitted: 8/26/17 12:00AM

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Article Title: Fluctuations When Driving Between Nonequilibrium Steady States

Authors: Paul M. Riechers, James P. Crutchfield

Keywords: stochastic thermodynamics, fluctuation theorem, nonequilibrium, neuronal ion channel

Abstract: Maintained by environmental fluxes, biological systems are thermodynamic processes that operate far from equilibrium without detailed-balanced dynamics. Yet, they often exhibit well defined nonequilibrium steady states (NESSs). More importantly, critical thermodynamic functionality arises directly from transitions among their NESSs, driven by environmental switching. Here, we identify the constraints on excess heat and dissipated work necessary to control a system that is kept far from equilibrium by background, uncontrolled "housekeeping" forces. We do this by extending the Crooks fluctuation theorem to transitions among NESSs, without invoking an unphysical dual dynamics. This and corresponding integral fluctuation theorems determine how much work must be expended when controlling systems maintained far from equilibrium. This generalizes thermodynamic feedback control theory, showing that Maxwellian Demons can leverage mesoscopic-state information to take advantage of the ...

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Journal: Physical Review E

Publication Identifier Type: DOI

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Date Submitted: 8/26/17 12:00AM

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Publication Location:

Article Title: Minimum memory for generating rare events

Authors: Cina Aghamohammadi, James P. Crutchfield

Keywords: stochastic processes, large deviation theory, computational mechanics, fluctuation spectra

Abstract: We classify the rare events of structured, memoryful stochastic processes and use this to analyze sequential and parallel generators for these events. Given a stochastic process, we introduce a method to construct a new process whose typical realizations are a given process' rare events. This leads to an expression for the minimum memory required to generate rare events. We then show that the recently discovered classical-quantum ambiguity of simplicity also occurs when comparing the structure of process fluctuations.

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Article Title: Leveraging Environmental Correlations: The Thermodynamics of Requisite Variety

Authors: Alexander B. Boyd, Dibyendu Mandal, James P. Crutchfield

Keywords: Maxwell's Demon, cybernetics, detailed balance, entropy rate, Second Law of Thermodynamics, transducer, adaptation

Abstract: Key to biological success, the requisite variety that confronts an adaptive organism is the set of detectable, accessible, and controllable states in its environment. We analyze its role in the thermodynamic functioning of information ratchets—a form of autonomous Maxwellian Demon capable of exploiting fluctuations in an external information reservoir to harvest useful work from a thermal bath. This establishes a quantitative paradigm for understanding how adaptive agents leverage structured thermal environments for their own thermodynamic benefit. General ratchets behave as memoryful communication channels, interacting with their environment sequentially and storing results to an output. The bulk of thermal ratchets analyzed to date, however, assume memoryless environments that generate input signals without temporal correlations. Employing computational mechanics and a new information-processing Second Law of Thermodynamics (IPSL) we ...

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Article Title: Extreme Quantum Advantage when Simulating Classical Systems with Long-Range Interaction

Authors: Cina Aghamohammadi, John R. Mahoney, James P. Crutchfield

Keywords: stochastic process, Ising model, Dyson model, long-range interaction, strongly correlated system, quantum information, quantum communication, quantum complexity, quantum machine, statistical complexity

Abstract: Classical stochastic processes can be generated by quantum simulators instead of the more standard classical ones, such as hidden Markov models. One reason for using quantum simulators has recently come to the fore: they generally require less memory than their classical counterparts. Here, we examine this quantum advantage for strongly coupled spin systems—in particular, the Dyson one-dimensional Ising spin chain with variable interaction length. We find that the advantage scales with both interaction range and temperature, growing without bound as interaction range increases. In particular, simulating Dyson's original spin chain with the most memory-efficient classical algorithm known requires infinite memory, while a quantum simulator requires only finite memory. Thus, quantum systems can very efficiently simulate strongly coupled one-dimensional classical spin systems.

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Journal: Physical Review E
Publication Identifier Type: DOI **Publication Identifier:** 10.1103/PhysRevE.95.012152
Volume: 95 **Issue:** 1 **First Page #:** 012152-1
Date Submitted: 8/26/17 12:00AM **Date Published:** 1/1/17 4:00PM
Publication Location:

Article Title: Correlation-powered information engines and the thermodynamics of self-correction

Authors: Alexander B. Boyd, Dibyendu Mandal, James P. Crutchfield

Keywords: Maxwell's Demon, Maxwell's refrigerator, detailed balance, entropy rate, Second Law of Thermodynamics

Abstract: Information engines can use structured environments as a resource to generate work by randomizing ordered inputs and leveraging the increased Shannon entropy to transfer energy from a thermal reservoir to a work reservoir. We give a broadly applicable expression for the work production of an information engine, generally modeled as a memoryful channel that communicates inputs to outputs as it interacts with an evolving environment. The expression establishes that an information engine must have more than one memory state in order to leverage input environment correlations. To emphasize this functioning, we designed an information engine powered solely by temporal correlations and not by statistical biases, as employed by previous engines. Key to this is the engine's ability to synchronize—the engine automatically returns to a desired dynamical phase when thrown into an unwanted, dissipative phase by corruptions in the input—that is, by unanticipated environmental fluctuations. ...

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Journal: Physics Letters A
Publication Identifier Type: DOI **Publication Identifier:** 10.1016/j.physleta.2016.12.036
Volume: 381 **Issue:** 14 **First Page #:** 1223
Date Submitted: 8/26/17 12:00AM **Date Published:** 4/1/17 7:00AM
Publication Location:

Article Title: The Ambiguity of Simplicity in Quantum and Classical Simulation

Authors: Cina Aghamohammadi, John R. Mahoney, James P. Crutchfield

Keywords: quantum information, information theory, stochastic process, hidden Markov model, ?-machine

Abstract: A system's perceived simplicity depends on whether it is represented classically or quantumly. This is not so surprising, as classical and quantum physics are descriptive frameworks built on different assumptions that capture, emphasize, and express different properties and mechanisms. What is surprising is that, as we demonstrate, simplicity is ambiguous: the relative simplicity between two systems can change sign when moving between classical and quantum descriptions. Here, we associate simplicity with small model-memory. We see that the notions of absolute physical simplicity at best form a partial, not a total, order. This suggests that appeals to principles of physical simplicity, via Ockham's Razor or to the "elegance" of competing theories, may be fundamentally subjective. Recent rapid progress in quantum computation and quantum simulation suggest that the ambiguity of simplicity will strongly impact statistical inference and, in particular, model selection.

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Volume: 116 **Issue:** 23 **First Page #:** 238701-1
Date Submitted: 8/26/17 12:00AM **Date Published:** 6/1/16 7:00AM
Publication Location:
Article Title: Information Flows? A Critique of Transfer Entropies
Authors: Ryan G. James, Nix Barnett, James P. Crutchfield
Keywords: stochastic process, transfer entropy, causation entropy, partial information decomposition, network science
Abstract: A central task in analyzing complex dynamics is to determine the loci of information storage and the communication topology of information flows within a system. Over the last decade and a half, diagnostics for the latter have come to be dominated by the transfer entropy. Via straightforward examples, we show that it and a derivative quantity, the causation entropy, do not, in fact, quantify the flow of information. At one and the same time they can overestimate flow or underestimate influence. We isolate why this is the case and propose several avenues to alternate measures for information flow. We also address an auxiliary consequence: The proliferation of networks as a now-common theoretical model for large-scale systems, in concert with the use of transferlike entropies, has shoehorned dyadic relationships into our structural interpretation of the organization and behavior of complex systems. This interpretation thus fails to include the effects of polyadic dependencies. ...
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Journal: Physics Letters A
Publication Identifier Type: DOI **Publication Identifier:** 10.1016/j.physleta.2016.02.052
Volume: 380 **Issue:** 17 **First Page #:** 1517
Date Submitted: 8/26/17 12:00AM **Date Published:** 4/1/16 2:00PM
Publication Location:
Article Title: Statistical signatures of structural organization: The case of long memory in renewal processes
Authors: Sarah E. Marzen, James P. Crutchfield
Keywords: stationary renewal process, fractal renewal process, statistical complexity, excess entropy, long memory, power-law scaling, 1/f noise, Zipf's law
Abstract: Identifying and quantifying memory are often critical steps in developing a mechanistic understanding of stochastic processes. These are particularly challenging and necessary when exploring processes that exhibit long-range correlations. The most common signatures employed rely on second-order temporal statistics and lead, for example, to identifying long memory in processes with power-law autocorrelation function and Hurst exponent greater than 1/2. However, most stochastic processes hide their memory in higher-order temporal correlations. Information measures—specifically, divergences in the mutual information between a process' past and future (excess entropy) and minimal predictive memory stored in a process' causal states (statistical complexity)—provide a different way to identify long memory in processes with higher-order temporal correlations. However, ...
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Publication Location:

Article Title: Minimized state complexity of quantum-encoded cryptic processes

Authors: Paul M. Riechers, John R. Mahoney, Cina Aghamohammadi, James P. Crutchfield

Keywords: stochastic process, hidden Markov model, ?-machine, causal states, mutual information, information compression, quantum state overlap, crypticity, spectral decomposition

Abstract: The predictive information required for proper trajectory sampling of a stochastic process can be more efficiently transmitted via a quantum channel than a classical one. This recent discovery allows quantum information processing to drastically reduce the memory necessary to simulate complex classical stochastic processes. It also points to a new perspective on the intrinsic complexity that nature must employ in generating the processes we observe. The quantum advantage increases with codeword length: the length of process sequences used in constructing the quantum communication scheme. In analogy with the classical complexity measure, statistical complexity, we use this reduced communication cost as an entropic measure of state complexity in the quantum representation. Previously difficult to compute, the quantum advantage is expressed here in closed form using spectral decomposition. ...

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Journal: Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences
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Volume: 374 **Issue:** 2063 **First Page #:** 20150067
Date Submitted: 8/26/17 12:00AM **Date Published:** 2/1/16 4:00PM
Publication Location:

Article Title: What did Erwin mean? The physics of information from the materials genomics of aperiodic crystals and water to molecular information catalysts and life

Authors: D. P. Varn, J. P. Crutchfield

Keywords: entropy, randomness, disorder, structure, mutual information, Maxwell's Demon

Abstract: Erwin Schro?dinger famously and presciently ascribed the vehicle transmitting the hereditary information underlying life to an 'aperiodic crystal'. We compare and contrast this, only later discovered to be stored in the linear biomolecule DNA, with the information-bearing, layered quasi-one-dimensional materials investigated by the emerging field of chaotic crystallography. Despite differences in functionality, the same information measures capture structure and novelty in both, suggesting an intimate coherence between the information character of biotic and abiotic matter—a broadly applicable physics of information. We review layered solids and consider three examples of how information- and computation-theoretic techniques are being applied to understand their structure. In particular, (i) we review recent efforts to apply new kinds of information measures to quantify disordered crystals; (ii) we discuss the structure of ice I in information-theoretic terms; and (iii) we ...

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Date Submitted: 8/26/17 12:00AM

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Publication Location:

Article Title: Occam's Quantum Strop: Synchronizing and Compressing Classical Cryptic Processes via a Quantum Channel

Authors: John R. Mahoney, Cina Aghamohammadi, James P. Crutchfield

Keywords: epsilon-machine, synchronization, compression, communication channel, quantum state overlap, von Neumann entropy, Shannon entropy rate, excess entropy, unifilarity

Abstract: A stochastic process' statistical complexity stands out as a fundamental property: the minimum information required to synchronize one process generator to another. How much information is required, though, when synchronizing over a quantum channel? Recent work demonstrated that representing causal similarity as quantum state-indistinguishability provides a quantum advantage. We generalize this to synchronization and offer a sequence of constructions that exploit extended causal structures, finding substantial increase of the quantum advantage. We demonstrate that maximum compression is determined by the process' cryptic order—a classical, topological property closely allied to Markov order, itself a measure of historical dependence. We introduce an efficient algorithm that computes the quantum advantage and close noting that the advantage comes at a cost—one trades off prediction for generation complexity.

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Date Submitted: 8/26/17 12:00AM

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Publication Location:

Article Title: Identifying functional thermodynamics in autonomous Maxwellian ratchets

Authors: Alexander B Boyd, Dibyendu Mandal, James P Crutchfield

Keywords: Maxwell's Demon, Maxwell's refrigerator, detailed balance, entropy rate, Second Law of Thermodynamics

Abstract: We introduce a family of Maxwellian Demons for which correlations among information bearing degrees of freedom can be calculated exactly and in compact analytical form. This allows one to precisely determine Demon functional thermodynamic operating regimes, when previous methods either misclassify or simply fail due to approximations they invoke. This reveals that these Demons are more functional than previous candidates. They too behave either as engines, lifting a mass against gravity by extracting energy from a single heat reservoir, or as Landauer erasers, consuming external work to remove information from a sequence of binary symbols by decreasing their individual uncertainty. Going beyond these, our Demon exhibits a new functionality that erases bits not by simply decreasing individual-symbol uncertainty, but by increasing inter-bit correlations (that is, by adding temporal order) while increasing single-symbol uncertainty. In all cases, but especially in the new erasure ...

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Date Submitted: 8/26/17 12:00AM

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Publication Location:

Article Title: The Elusive Present: Hidden Past and Future Dependency and Why We Build Models

Authors: Pooneh M. Ara, Ryan G. James, James P. Crutchfield

Keywords: stochastic process, hidden Markov model, causal shielding, ϵ -machine, causal states, mutual information

Abstract: Modeling a temporal process as if it is Markovian assumes the present encodes all of a process's history. When this occurs, the present captures all of the dependency between past and future. We recently showed that if one randomly samples in the space of structured processes, this is almost never the case. So, how does the Markov failure come about? That is, how do individual measurements fail to encode the past? And, how many are needed to capture dependencies between the past and future? Here, we investigate how much information can be shared between the past and future, but not be reflected in the present. We quantify this elusive information, give explicit calculational methods, and draw out the consequences. The most important of which is that when the present hides past-future correlation or dependency we must move beyond sequence-based statistics and build state-based models.

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Volume: 116

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Publication Location:

Article Title: Maxwell Demon Dynamics: Deterministic Chaos, the Szilard Map, and the Intelligence of Thermodynamic Systems

Authors: Alexander B. Boyd, James P. Crutchfield

Keywords: deterministic chaos, Lyapunov characteristic exponents, Markov partition, Landauer's Principle, measurement, erasure, memory, entropy rate, mutual information, dissipated work, control theory

Abstract: We introduce a deterministic chaotic system—the Szilard map—that encapsulates the measurement, control, and erasure protocol by which Maxwellian demons extract work from a heat reservoir. Implementing the demon's control function in a dynamical embodiment, our construction symmetrizes the demon and the thermodynamic system, allowing one to explore their functionality and recover the fundamental trade-off between the thermodynamic costs of dissipation due to measurement and those due to erasure. The map's degree of chaos—captured by the Kolmogorov-Sinai entropy—is the rate of energy extraction from the heat bath. Moreover, an engine's statistical complexity quantifies the minimum necessary system memory for it to function. In this way, dynamical instability in the control protocol plays an essential and constructive role in intelligent thermodynamic systems.

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Article Title: Predictive Rate-Distortion for Infinite-Order Markov Processes

Authors: Sarah E. Marzen, James P. Crutchfield

Keywords: Optimal causal filtering, Computational mechanics, Epsilon-machine, Causal states, Predictive rate-distortion, Information bottleneck

Abstract: Predictive rate-distortion analysis suffers from the curse of dimensionality: clustering arbitrarily long pasts to retain information about arbitrarily long futures requires resources that typically grow exponentially with length. The challenge is compounded for infinite-order Markov processes, since conditioning on finite sequences cannot capture all of their past dependencies. Spectral arguments confirm a popular intuition: algorithms that cluster finite-length sequences fail dramatically when the underlying process has long-range temporal correlations and can fail even for processes generated by finite-memory hidden Markov models. We circumvent the curse of dimensionality in rate-distortion analysis of finite- and infinite-order processes by casting predictive rate-distortion objective functions in terms of the forward- and reverse-time causal states of computational mechanics. Examples demonstrate that the resulting algorithms yield substantial improvements.

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Article Title: Exact complexity: The spectral decomposition of intrinsic computation

Authors: James P. Crutchfield, Christopher J. Ellison, Paul M. Riechers

Keywords: Excess entropy, Statistical complexity, Projection operator, Resolvent, Entropy rate, Predictable information

Abstract: We give exact formulae for a wide family of complexity measures that capture the organization of hidden nonlinear processes. The spectral decomposition of operator-valued functions leads to closed-form expressions involving the full eigenvalue spectrum of the mixed-state presentation of a process's ϵ -machine causal-state dynamic. Measures include correlation functions, power spectra, past-future mutual information, transient and synchronization informations, and many others. As a result, a direct and complete analysis of intrinsic computation is now available for the temporal organization of finitary hidden Markov models and nonlinear dynamical systems with generating partitions and for the spatial organization in one-dimensional systems, including spin systems, cellular automata, and complex materials via chaotic crystallography.

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Volume: 8

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Publication Location:

Article Title: Thermodynamics of Modularity: Structural Costs Beyond the Landauer Bound

Authors: A. B. Boyd, D. Mandal, and J. P. Crutchfield

Keywords: Transducer, intrinsic computation, informational Second Law of Thermodynamics

Abstract: Information processing typically occurs via the composition of modular units, such as the universal logic gates found in discrete computation circuits. The benefit of modular information processing, in contrast to globally integrated information processing, is that complex computations are more easily and flexibly implemented via a series of simpler, localized information processing operations that only control and change local degrees of freedom. We show that, despite these benefits, there are unavoidable thermodynamic costs to modularity—costs that arise directly from the operation of localized processing and that go beyond Landauer's bound on the work required to erase information. Localized operations are unable to leverage global correlations, which are a thermodynamic fuel. We quantify the minimum irretrievable dissipation of modular computations in terms of the difference between the change in global nonequilibrium free energy, which captures these global correlations, and ...

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Date Submitted: 8/18/18 12:00AM

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Publication Location:

Article Title: Prediction and Generation of Binary Markov Processes: Can a Finite-State Fox Catch a Markov Mouse?

Authors: J. Ruebeck, R. G. James, J. R. Mahoney, J. P. Crutchfield

Keywords: stochastic process, hidden Markov model, ?-machine, causal states, mutual information

Abstract: Understanding the generative mechanism of a natural system is a vital component of the scientific method. Here, we investigate one of the fundamental steps toward this goal by presenting the minimal generator of an arbitrary binary Markov process. This is a class of processes whose predictive model is well known. Surprisingly, the generative model requires three distinct topologies for different regions of parameter space. We show that a previously proposed generator for a particular set of binary Markov processes is, in fact, not minimal. Our results shed the first quantitative light on the relative (minimal) costs of prediction and generation. We find, for instance, that the difference between prediction and generation is maximized when the process is approximately independently, identically distributed.

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Date Submitted: 8/18/18 12:00AM

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Publication Location:

Article Title: Extreme Quantum Advantage for Rare-Event Sampling

Authors: C. Aghamohammadi, S. P. Loomis, J. R. Mahoney, J. P. Crutchfield

Keywords: quantum algorithm, large deviation theory, biased sampling, quantum memory, quantum advantage, stochastic process, hidden Markov model

Abstract: We introduce a quantum algorithm for efficient biased sampling of the rare events generated by classical memoryful stochastic processes. We show that this quantum algorithm gives an extreme advantage over known classical biased sampling algorithms in terms of the memory resources required. The quantum memory advantage ranges from polynomial to exponential and when sampling the rare equilibrium configurations of spin systems the quantum advantage diverges.

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Publication Location:

Article Title: Spectral Simplicity of Apparent Complexity, Part II: Exact Complexities and Complexity Spectra

Authors: P. M. Riechers, J. P. Crutchfield

Keywords: hidden Markov model, entropy rate, excess entropy, predictable information, statistical complexity, projection operator, complex analysis, resolvent, Drazin inverse

Abstract: The meromorphic functional calculus developed in Part I overcomes the nondiagonalizability of linear operators that arises often in the temporal evolution of complex systems and is generic to the metadynamics of predicting their behavior. Using the resulting spectral decomposition, we derive closed-form expressions for correlation functions, finite-length Shannon entropy-rate approximates, asymptotic entropy rate, excess entropy, transient information, transient and asymptotic state uncertainty, and synchronization information of stochastic processes generated by finite-state hidden Markov models. This introduces analytical tractability to investigating information processing in discrete-event stochastic processes, symbolic dynamics, and chaotic dynamical systems. Comparisons reveal mathematical similarities between complexity measures originally thought to capture distinct informational and computational properties. We also introduce a new kind of spectral analysis via

...

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Journal: Chaos

Publication Identifier Type: DOI

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Volume: 28

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Date Submitted: 8/18/18 12:00AM

Date Published: 7/10/17 7:26AM

Publication Location:

Article Title: Spectral Simplicity of Apparent Complexity, Part I: The Nondiagonalizable Metadynamics of Prediction

Authors: P. M. Riechers, J. P. Crutchfield

Keywords: hidden Markov model, entropy rate, excess entropy, predictable information, statistical complexity, projection operator, complex analysis, resolvent, Drazin inverse

Abstract: Virtually all questions that one can ask about the behavioral and structural complexity of a stochastic process reduce to a linear algebraic framing of a time evolution governed by an appropriate hidden-Markov process generator. Each type of question—correlation, predictability, predictive cost, observer synchronization, and the like—induces a distinct generator class. Answers are then functions of the class-appropriate transition dynamic. Unfortunately, these dynamics are generally nonnormal, nondiagonalizable, singular, and so on. Tractably analyzing these dynamics relies on adapting the recently introduced meromorphic functional calculus, which specifies the spectral decomposition of functions of nondiagonalizable linear operators, even when the function poles and zeros coincide with the operator's spectrum. Along the way, we establish special properties of the projection operators that demonstrate how they capture the organization of subprocesses within a complex system. ...

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Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published

Journal: Entropy

Publication Identifier Type: DOI

Publication Identifier: 10.3390/e19100531

Volume: 19

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Date Submitted: 8/18/18 12:00AM

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Publication Location:

Article Title: Multivariate Dependence Beyond Shannon Information

Authors: R. G. James, J. P. Crutchfield

Keywords: stochastic process, transfer entropy, causation entropy, partial information decomposition, network science, causality

Abstract: Accurately determining dependency structure is critical to discovering a system's causal organization. We recently showed that the transfer entropy fails in a key aspect of this—measuring information flow—due to its conflation of dyadic and polyadic relationships. We extend this observation to demonstrate that this is true of all such Shannon information measures when used to analyze multivariate dependencies. This has broad implications, particularly when employing information to express the organization and mechanisms embedded in complex systems, including the burgeoning efforts to combine complex network theory with information theory. Here, we do not suggest that any aspect of information theory is wrong. Rather, the vast majority of its informational measures are simply inadequate for determining the meaningful dependency structure within joint probability distributions. Therefore, such information measures are inadequate for discovering intrinsic causal relations. ...

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Volume: 8

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Date Submitted: 9/2/19 12:00AM

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Publication Location:

Article Title: Beyond the Spectral Theorem: Spectrally Decomposing Arbitrary Functions of Nondiagonalizable Operators

Authors: P. M. Riechers, J. P. Crutchfield

Keywords: functional calculus, linear operator, projection operator, eigenspectrum

Abstract: Nonlinearities in finite dimensions can be linearized by projecting them into infinite dimensions. Unfortunately, often the linear operator techniques that one would then use simply fail since the operators cannot be diagonalized. This curse is well known. It also occurs for finite-dimensional linear operators. We circumvent it by developing a meromorphic functional calculus that can decompose arbitrary functions of nondiagonalizable linear operators in terms of their eigenvalues and projection operators. It extends the spectral theorem of normal operators to a much wider class, including circumstances in which poles and zeros of the function coincide with the operator spectrum. By allowing the direct manipulation of individual eigenspaces of nonnormal and nondiagonalizable operators, the new theory avoids spurious divergences. As such, it yields novel insights and closed-form expressions across several areas of physics in which nondiagonalizable dynamics are relevant, ...

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Journal: PHYSICAL REVIEW LETTERS

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Publication Identifier: 10.1103/PhysRevLett.119.258001

Volume: 119

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First Page #: 258001

Date Submitted: 8/28/18 12:00AM

Date Published:

Publication Location:

Article Title: Entropy production and fluctuation theorems for active matter

Authors: Dibyendu Mandal, K. Klymko, Michael R. DeWeese

Keywords: active matter, nonequilibrium, entropy, stochastic thermodynamics, free energy

Abstract: Active biological systems reside far from equilibrium, dissipating heat even in their steady state, thus requiring an extension of conventional equilibrium thermodynamics and statistical mechanics. In this Letter, we have extended the emerging framework of stochastic thermodynamics to active matter. In particular, for the active Ornstein-Uhlenbeck model, we have provided consistent definitions of thermodynamic quantities such as work, energy, heat, entropy, and entropy production at the level of single, stochastic trajectories and derived related fluctuation relations. We have developed a generalization of the Clausius inequality, which is valid even in the presence of the non-Hamiltonian dynamics underlying active matter systems. We have illustrated our results with explicit numerical studies.

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Publication Location:

Article Title: Near-optimal protocols in complex nonequilibrium transformations

Authors: Todd R. Gingrich, Grant M. Rotskoff, Gavin E. Crooks, Phillip L. Geissler

Keywords: nonequilibrium, free energy, entropy, Ising model, optimization

Abstract: The development of sophisticated experimental means to control nanoscale systems has motivated efforts to design driving protocols that minimize the energy dissipated to the environment. Computational models are a crucial tool in this practical challenge. We describe a general method for sampling an ensemble of finite-time, nonequilibrium protocols biased toward a low average dissipation. We show that this scheme can be carried out very efficiently in several limiting cases. As an application, we sample the ensemble of low-dissipation protocols that invert the magnetization of a 2D Ising model and explore how the diversity of the protocols varies in response to constraints on the average dissipation. In this example, we find that there is a large set of protocols with average dissipation close to the optimal value, which we argue is a general phenomenon.

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Journal: JOURNAL OF CHEMICAL PHYSICS

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Publication Identifier: 10.1063/1.4997091

Volume: 147

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Date Submitted: 8/28/18 12:00AM

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Publication Location:

Article Title: Statistical mechanics of transport processes in active fluids: Equations of hydrodynamics

Authors: Katherine Klymko, Dibyendu Mandal, Kranthi K. Mandadapu

Keywords: Active matter; continuum mechanics; polar hydrodynamics; transport phenomena; Irving-Kirkwood procedure; asymmetric stress tensor

Abstract: The equations of hydrodynamics including mass, linear momentum, angular momentum, and energy are derived by coarse-graining the microscopic equations of motion for systems consisting of rotary dumbbells driven by internal torques. In deriving the balance of linear momentum, we find that the symmetry of the stress tensor is broken due to the presence of non-zero torques on individual particles. The broken symmetry of the stress tensor induces internal spin in the fluid and leads us to consider the balance of internal angular momentum in addition to the usual moment of momentum. In the absence of spin, the moment of momentum is the same as the total angular momentum. In deriving the form of the balance of total angular momentum, we find the microscopic expressions for the couple stress tensor that drives the spin field. We show that the couple stress contains contributions from both intermolecular interactions and the active forces. The presence of spin leads to the idea of balance ...

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Journal: The Journal of Physical Chemistry B

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Volume: 121

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Date Submitted: 8/29/17 12:00AM

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Publication Location:

Article Title: Classical and Quantum Shortcuts to Adiabaticity in a Tilted Piston

Authors: Ayoti Patra, Christopher Jarzynski

Keywords: shortcuts to adiabaticity, semiclassical approximations

Abstract: We constructed and investigated an exactly solvable model system for which a quantum counterdiabatic (CD) Hamiltonian was obtained directly from its classical counterpart. Previously this had been accomplished only for scale-invariant Hamiltonians. Using numerical solutions of the time-dependent Schrödinger equation, we verified that our CD term effectively suppresses non-adiabatic excitations.

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Date Published: 3/1/17 4:00PM

Publication Location:

Article Title: Fast forward to the classical adiabatic invariant

Authors: Christopher Jarzynski, Sebastian Deffner, Ayoti Patra, Yi?it Suba??

Keywords: shortcuts to adiabaticity, dynamical systems

Abstract: We show how the classical action, an adiabatic invariant, can be preserved under nonadiabatic conditions. Specifically, for a time-dependent Hamiltonian $H = p^2/2m + U(q,t)$ in one degree of freedom, and for an arbitrary choice of action I_0 , we construct a so-called fast-forward potential energy function $FF(q,t)$ that, when added to H , guides all trajectories with initial action I_0 to end with the same value of action. We use this result to construct a local dynamical invariant $J(q,p,t)$ whose value remains constant along these trajectories. We illustrate our results with numerical simulations. Finally, we sketch how our classical results may be used to design approximate quantum shortcuts to adiabaticity.

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Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published

Journal: New Journal of Physics

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Volume: 19

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Date Submitted: 8/27/18 12:00AM

Date Published: 7/28/17 1:56AM

Publication Location:

Article Title: Shortcuts to adiabaticity using flow fields

Authors: A. Patra, C. Jarzynski

Keywords: shortcuts to adiabaticity, engineered swift equilibration

Abstract: A shortcut to adiabaticity is a recipe for generating adiabatic evolution at an arbitrary pace. Shortcuts have been developed for quantum, classical and (most recently) stochastic dynamics. A shortcut might involve a counterdiabatic Hamiltonian that causes a system to follow the adiabatic evolution at all times, or it might utilize a fast-forward potential, which returns the system to the adiabatic path at the end of the process. We develop a general framework for constructing shortcuts to adiabaticity from flow fields that describe the desired adiabatic evolution. Our approach encompasses quantum, classical and stochastic dynamics, and provides surprisingly compact expressions for both counterdiabatic Hamiltonians and fast-forward potentials. We illustrate our method with numerical simulations of a model system, and we compare our shortcuts with previously obtained results. We also consider the semiclassical connections between our quantum and classical shortcuts. Our method, ...

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Volume: 169

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Date Published: 8/1/17 7:00AM

Publication Location:

Article Title: Structure and Randomness of Continuous-Time, Discrete-Event Processes

Authors: Sarah E. Marzen, James P. Crutchfield

Keywords: Epsilon-machines, Causal states, Entropy rate, Statistical complexity, Hidden Markov processes

Abstract: Loosely speaking, the Shannon entropy rate is used to gauge a stochastic process' intrinsic randomness; the statistical complexity gives the cost of predicting the process. We calculate, for the first time, the entropy rate and statistical complexity of stochastic processes generated by finite unifilar hidden semi-Markov models—memoryful, state-dependent versions of renewal processes. Calculating these quantities requires introducing novel mathematical objects (epsilon-machines of hidden semi-Markov processes) and new information-theoretic methods to stochastic processes.

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Journal: Physical Review X

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Date Submitted: 8/18/18 12:00AM

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Publication Location:

Article Title: Causal Asymmetry in a Quantum World

Authors: Jayne Thompson, Andrew J. P. Garner, John R. Mahoney, James P. Crutchfield, Vlatko Vedral, Mile Gu

Keywords: Quantum Physics, Quantum Information

Abstract: Causal asymmetry is one of the great surprises in predictive modeling: The memory required to predict the future differs from the memory required to retrodict the past. There is a privileged temporal direction for modeling a stochastic process where memory costs are minimal. Models operating in the other direction incur an unavoidable memory overhead. Here, we show that this overhead can vanish when quantum models are allowed. Quantum models forced to run in the less-natural temporal direction not only surpass their optimal classical counterparts but also any classical model running in reverse time. This holds even when the memory overhead is unbounded, resulting in quantum models with unbounded memory advantage.

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Journal: Chaos: An Interdisciplinary Journal of Nonlinear Science

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Volume: 28

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Date Submitted: 8/18/18 12:00AM

Date Published: 7/1/18 7:00AM

Publication Location:

Article Title: Local causal states and discrete coherent structures

Authors: Adam Rupe, James P. Crutchfield

Keywords: coherent structures, spatially extended dynamical systems, emergence, symmetry breaking, cellular automata

Abstract: Coherent structures form spontaneously in nonlinear spatiotemporal systems and are found at all spatial scales in natural phenomena from laboratory hydrodynamic flows and chemical reactions to ocean, atmosphere, and planetary climate dynamics. Phenomenologically, they appear as key components that organize the macroscopic behaviors in such systems. Despite a century of effort, they have eluded rigorous analysis and empirical prediction, with progress being made only recently. As a step in this, we present a formal theory of coherent structures in fully discrete dynamical field theories. It builds on the notion of structure introduced by computational mechanics, generalizing it to a local spatiotemporal setting. The analysis' main tool employs the local causal states, which are used to uncover a system's hidden spatiotemporal symmetries and which identify coherent structures as spatially localized deviations from those symmetries. The approach is behavior-driven in the sense that...

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Date Submitted: 8/18/18 12:00AM

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Publication Location:

Article Title: Optimized bacteria are environmental prediction engines

Authors: Sarah E. Marzen, James P. Crutchfield

Keywords: bet hedging, isogenic bacteria, causal states, epigenetic states

Abstract: Experimentalists observe phenotypic variability even in isogenic bacteria populations. We explore the hypothesis that in fluctuating environments this variability is tuned to maximize a bacterium's expected log-growth rate, potentially aided by epigenetic (all inheritable nongenetic) markers that store information about past environments. Crucially, we assume a time delay between sensing and action, so that a past epigenetic marker is used to generate the present phenotypic variability. We show that, in a complex, memoryful environment, the maximal expected log-growth rate is linear in the instantaneous predictive information—the mutual information between a bacterium's epigenetic markers and future environmental states. Hence, under resource constraints, optimal epigenetic markers are causal states—the minimal sufficient statistics for prediction—or lossy approximations thereof. We propose new theoretical investigations into and new experiments on bacteria phenotypic bet-hedging ...

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Volume: Issue:

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Date Submitted: 9/2/19 12:00AM

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Publication Location:

Article Title: Unique Information via Dependency Constraints

Authors: R. G. James, J. Emenhesier, and J. P. Crutchfield

Keywords: partial information decomposition, mutual information, statistical dependence, information theory, cybernetics

Abstract: The partial information decomposition is perhaps the leading proposal for resolving shared information in a joint random variable into redundant, synergistic, and unique constituents. Unfortunately, the framework has been hindered by a lack of a generally agreed-upon, multivariate method of quantifying the constituents. Here, we take a step toward rectifying this by developing a decomposition based on a new method that quantifies unique information. The result is the first measure that satisfies the core axioms of the framework while also not treating statistically identical but independent channels as redundant. This marks a key step forward in the practical application of the partial information decomposition.

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Volume: Issue:

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Date Published: 5/13/18 6:16PM

Publication Location: Boulder, Colorado

Article Title: A Physics-Based Approach to Unsupervised Discovery of Coherent Structures in Spatiotemporal Systems

Authors: A. Rupe, J. P. Crutchfield, K. Kashinath, Prabhat

Keywords: local causal states, light cone reconstruction

Abstract: Given that observational and numerical climate data are being produced at ever more prodigious rates, increasingly sophisticated and automated analysis techniques have become essential. Deep learning is quickly becoming a standard approach for such analyses and, while great progress is being made, major challenges remain. Unlike commercial applications in which deep learning has led to surprising successes, scientific data is highly complex and typically unlabeled. Moreover, interpretability and detecting new mechanisms are key to scientific discovery. To enhance discovery we present a complementary physics-based, data-driven approach that exploits the causal nature of spatiotemporal data sets generated by local dynamics (e.g. hydrodynamic flows). We illustrate how novel patterns and coherent structures can be discovered in cellular automata and outline the path from them to climate data.

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Date Submitted: 8/21/18 12:00AM

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Publication Location:

Article Title: Inter-scale information flow as a surrogate for downward causation that maintains spiral waves

Authors: Hiroshi Ashikaga, Ryan G. James

Keywords: reaction-diffusion, pattern formation, information measures

Abstract: A rotor, the rotation center of spiral waves, has been proposed as a causal mechanism to maintain atrial fibrillation (AF) in human. However, our current understanding of the causality between rotors and spiral waves remains incomplete. One approach to improving our understanding is to determine the relationship between rotors and downward causation from the macro-scale collective behavior of spiral waves to the micro-scale behavior of individual components in a cardiac system. This downward causation is quantifiable as inter-scale information flow that can be used as a surrogate for the mechanism that maintains spiral waves. We used a numerical model of a cardiac system and generated a renormalization group with system descriptions at multiple scales. We found that transfer entropy quantified the upward and downward inter-scale information flow between micro- and macro-scale descriptions of the cardiac system with spiral waves. In addition, because the spatial profile of ...

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Journal: AIMS Journal

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Article Title: SUB-RIEMANNIAN GEOMETRY AND FINITE TIME THERMODYNAMICS PART 1: THE STOCHASTIC OSCILLATOR

Authors: Yunlong Huang and P. S. Krishnaprasad

Keywords: Geometric control, Maximum principle, Heat engine

Abstract: The field of sub-Riemannian geometry has flourished in the past four decades through the strong interactions between problems arising in applied science (in areas such as robotics) and questions of a pure mathematical character about the nature of space. Methods of control theory, such as controllability properties determined by Lie brackets of vector fields, the Hamilton equations associated to the Maximum Principle of optimal control, Hamilton-Jacobi-Bellman equation etc. have all been found to be basic tools for answering such questions. In this paper, we find a useful role for the vantage point of sub-Riemannian geometry in attacking a problem of interest in non-equilibrium statistical mechanics: how does one create rules for operation of micro- and nano-scale systems (heat engines) that are subject to fluctuations from the surroundings, so as to be able to do useful things such as converting heat into work over a cycle of operation? We exploit geometric optimal control the

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Journal: IRS Technical Report
Publication Identifier Type: Other **Publication Identifier:** ISR Technical Report 2018
Volume: **Issue:** **First Page #:**
Date Submitted: 8/26/18 12:00AM **Date Published:**
Publication Location:

Article Title: Optimal Control of KPZ Equation Using Deep Reinforcement Learning

Authors: Yunlong Huang, P. S. Krishnaprasad

Keywords: nonlinear stochastic partial differential equation, roughness, high-dimensional stochastic optimal control, curse of dimensionality

Abstract: The Kardar-Parisi-Zhang (KPZ) equation is a nonlinear stochastic partial differential equation which describes the temporal change of the height $h(x,t)$ of an interface at location x and time t . In this paper, we discuss the control of KPZ equation in one spatial dimension. One key problem of KPZ equation is to investigate the roughness of the interface. In a finite time duration, we would like to control the roughness by varying temperatures at different places. We first investigate the reachability of the control system to show that varying the temperatures at different locations will have effect on the variation of the heights of the interface. We then formulate the roughness minimization problem to be a high-dimensional stochastic optimal control problem. In order to cope with the well-known "curse of dimensionality" arising in the Hamilton-Jacobi-Bellman equation associated to an optimal control problem, we pursue an approach based on deep reinforcement learning. The application ..

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Journal: New Journal of Physics
Publication Identifier Type: Other **Publication Identifier:** New J Phys (2018)
Volume: in press **Issue:** **First Page #:**
Date Submitted: 8/28/18 12:00AM **Date Published:**
Publication Location:

Article Title: Similarities and Differences Between Nonequilibrium Steady States and Time-Periodic Driving in Diffusive Systems

Authors: D. M. Busiello, C. Jarzynski, and O. Raz

Keywords: stochastic pumping, nonequilibrium steady states

Abstract: A system that violates detailed balance evolves asymptotically into a nonequilibrium steady state with non-vanishing currents. Analogously, when detailed balance holds at any instant of time but the system is driven through time-periodic variations of external parameters, it evolves toward a time-periodic state, which can also support non-vanishing currents. In both cases the maintenance of currents throughout the system incurs a cost in terms of entropy production. Here we compare these two scenarios for one dimensional diffusive systems with periodic boundary condition, a framework commonly used to model biological and artificial molecular machines. We first show that the entropy production rate in a periodically driven system is necessarily greater than that in a stationary system without detailed balance, when both are described by the same (time-averaged) current and probability distribution. Next, we show how to construct both a non-equilibrium steady state and a periodic ...

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Volume: Issue:

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Publication Location:

Article Title: Strong and Weak Optimizations in Classical and Quantum Models of Stochastic Processes

Authors: Samuel Loomis, James P. Crutchfield

Keywords: hidden Markov models, stochastic process, λ -machine, Rényi-entropy, quantum Markov model, majorization, resource theory

Abstract: Among the predictive hidden Markov models that describe a given stochastic process, the λ -machine is strongly minimal in that it minimizes every Rényi-based memory measure. Quantum models can be smaller still. In contrast with the λ -machine's unique role in the classical setting, however, among the class of processes described by pure-state hidden quantum Markov models, there are those for which there does not exist any strongly minimal model. Quantum memory optimization then depends on which memory measure best matches a given problem circumstance.

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Journal: Public Library of Science One

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Article Title: On the sparse structure of natural sounds and natural images: similarities, differences, and implications for neural coding

Authors: Eric McVoy Dodds, Michael Robert DeWeese

Keywords: natural images, natural sounds, vision, audition, information theory, neural coding, sparse coding

Abstract: Sparse coding models of natural images and sounds have been able to predict several response properties of neurons in the visual and auditory systems. While the success of these models suggests that the structure they capture is universal across domains to some degree, it is not yet clear which aspects of this structure are universal and which vary across sensory modalities. To address this, we fit complete and highly overcomplete sparse coding models to natural images and spectrograms of speech and report on differences in the statistics learned by these models. We find several types of sparse features in natural images, which all appear in similar, approximately Laplacian distributions, whereas the many types of sparse features in speech exhibit a broad range of sparse distributions, many of which are highly asymmetric. Moreover, individual sparse coding units tend to exhibit higher lifetime sparseness for overcomplete models trained on images compared to those trained on speech ...

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Journal: Entropy

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Publication Location:

Article Title: Unique Information and Secret Key Agreement

Authors: Ryan James, Jeffrey Emenheiser, James Crutchfield

Keywords: information theory, partial information decomposition, secret key agreement, cryptography

Abstract: The partial information decomposition (PID) is a promising framework for decomposing a joint random variable into the amount of influence each source variable X_i has on a target variable Y , relative to the other sources. For two sources, influence breaks down into the information that both X_0 and X_1 redundantly share with Y , what X_0 uniquely shares with Y , what X_1 uniquely shares with Y , and finally what X_0 and X_1 synergistically share with Y . Unfortunately, considerable disagreement has arisen as to how these four components should be quantified. Drawing from cryptography, we consider the secret key agreement rate as an operational method of quantifying unique informations. Secret key agreement rate comes in several forms, depending upon which parties are permitted to communicate. We demonstrate that three of these four forms are inconsistent with the PID.

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Publication Location:

Article Title: dit: a Python package for discrete information theory

Authors: Ryan G. James, Christopher J. Ellison, James P. Crutchfield

Keywords: python, discrete information theory, open source

Abstract: dit--Dit: A python package for Discrete Information Theory, available at <https://github.com/dit/dit>--is a Python package for the study of discrete information theory. Information theory is a mathematical framework for the study of quantifying, compressing, and communicating random variables. More recently, information theory has been utilized within the physical and social sciences to quantify how different components of a system interact. dit is primarily concerned with this aspect of the theory.

Distribution Statement: 3-Distribution authorized to U.S. Government Agencies and their contractors

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RPPR Final Report as of 14-Jan-2021

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Journal: arxiv.org

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Publication Identifier: 10.1103/PhysRevE.102.040102

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Publication Location:

Article Title: Measurement-Induced Randomness and Structure in Controlled Qubit Processes

Authors: Ariadna E. Venegas-Li, Alexandra M. Jurgens, James P. Crutchfield

Keywords: measurement, quantum process, stochastic process

Abstract: Nonlinearities in finite dimensions can be linearized by projecting them into infinite dimensions.

Unfortunately, the familiar linear operator techniques that one would then use often fail since the operators cannot be diagonalized. This curse is well known. It also occurs for finite-dimensional linear operators. We circumvent it via two tracks. First, using the well-known holomorphic functional calculus, we develop new practical results about spectral projection operators and the relationship between left and right generalized eigenvectors. Second, we generalize the holomorphic calculus to a meromorphic functional calculus that can decompose arbitrary functions of nondiagonalizable linear operators in terms of their eigenvalues and projection operators. This simultaneously simplifies and generalizes functional calculus so that it is readily applicable to analyzing complex physical systems.

Distribution Statement: 1-Approved for public release; distribution is unlimited.

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Volume:

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Date Published:

Publication Location:

Article Title: Harnessing Fluctuations in Thermodynamic Computing via Time-Reversal Symmetries

Authors: G. Wimsatt, O.-P. Saira, A. B. Boyd, M. H. Matheny, S. Han, M. L. Roukes, J. P. Crutchfield

Keywords: Jarzynski integral fluctuation theorem, Crooks detailed fluctuation theorem, Landauer's Principle, thermodynamics of computation, information thermodynamics

Abstract: We experimentally demonstrate that highly structured distributions of work emerge during even the simple task of erasing a single bit. These are signatures of a refined suite of time-reversal symmetries in distinct functional classes of microscopic trajectories. As a consequence, we introduce a broad family of conditional fluctuation theorems that the component work distributions must satisfy. Since they identify entropy production, the component work distributions encode both the frequency of various mechanisms of success and failure during computing, as well giving improved estimates of the total irreversibly-dissipated heat. This new diagnostic tool provides strong evidence that thermodynamic computing at the nanoscale can be constructively harnessed. We experimentally verify this functional decomposition and the new class of fluctuation theorems by measuring transitions between flux states in a superconducting circuit.

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Journal: New Journal of Physics

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Date Submitted: 9/27/19 12:00AM

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Article Title: Similarities and differences between non-equilibrium steady states and time-periodic driving in diffusive systems

Authors: D M Busiello, C Jarzynski, O Raz

Keywords: periodic driving, nonequilibrium steady state, Fokker-Planck equation

Abstract: For diffusive evolution in one degree of freedom, we compare the thermodynamics of systems driven by time-periodic forcing ("stochastic pumps") with those driven by fixed forces that violate detailed balance. We prove that the entropy production in the former case is necessarily greater than that in the latter, when both are described by the same (time-averaged) current and probability distribution. We also show how to construct both a nonequilibrium steady state and a periodically driven state that support a given current and probability distribution.

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Publication Location:

Article Title: A Programmable Mechanical Maxwell's Demon

Authors: Zhiyue Lu, Christopher Jarzynski

Keywords: Maxwell's demon, Shannon entropy, information engine, Landauer's principle, Szilard engine, second law of thermodynamics

Abstract: We construct a mechanistic model of a device that acts as a Maxwellian demon, converting heat from a thermal bath into work to lift a mass against gravity. Our model is programmable: it can use as its input an arbitrary string of incoming bits, rather than (as in previous models) string in which all bits are set to the same state, 0 or 1. Our model can also act as a copying device, which uses the energy of a falling mass to copy information from a reference sequence of bits to a target sequence.

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Date Submitted: 9/27/19 12:00AM

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Article Title: Optimal Probabilistic Work Extraction beyond the Free Energy Difference with a Single-Electron Device

Authors: Olivier Maillet, Paolo A. Erdman, Vasco Cavina, Bibek Bhandari, Elsa T. Mannila, Joonas T. Peltonen, A

Keywords: work fluctuations, second law violations

Abstract: We argue theoretically and demonstrate experimentally that protocols can be constructed for which most realizations constitute nanoscale violations of the second law, i.e. the work performed on the system is less than the free energy difference between initial and final states: $W < \Delta F$. We also show that despite this feature, the average work continues to satisfy the second law: $\langle W \rangle \geq \Delta F$.

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Journal: Optics Express
Publication Identifier Type: DOI **Publication Identifier:** 10.1364/OE.27.014009
Volume: 27 **Issue:** 10 **First Page #:** 14009
Date Submitted: 9/27/19 12:00AM **Date Published:** 4/1/19 7:00AM
Publication Location:
Article Title: Design of optical neural networks with component imprecisions
Authors: Michael Y.-S. Fang, Sasikanth Manipatruni, Casimir Wierzynski, Amir Khosrowshahi, Michael R. DeWee
Keywords: optical neural networks, fault tolerance
Abstract: For the benefit of designing scalable, fault resistant optical neural networks (ONNs), we investigate the effects architectural designs have on the ONNs' robustness to imprecise components. We train two ONNs – one with a more tunable design (GridNet) and one with better fault tolerance (FFTNet) – to classify handwritten digits. When simulated without any imperfections, GridNet yields a better accuracy (?98%) than FFTNet (?95%). However, under a small amount of error in their photonic components, the more fault tolerant FFTNet overtakes GridNet. We further provide thorough quantitative and qualitative analyses of ONNs' sensitivity to varying levels and types of imprecisions. Our results offer guidelines for the principled design of fault-tolerant ONNs as well as a foundation for further research.
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CONFERENCE PAPERS:

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Date Received: 29-Aug-2016 **Conference Date:** 01-Jul-2015 **Date Published:**
Conference Location: Chicago, Illinois
Paper Title: Station Keeping through Beacon-referenced Cyclic Pursuit
Authors: Kevin S. Galloway, Biswadip Dey
Acknowledged Federal Support: N

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Conference Name: 2015 American Control Conference
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Authors:
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Conference Name: 2016 American Control Conference
Date Received: 29-Aug-2016 **Conference Date:** 06-Jul-2016 **Date Published:** 15-Jul-2016
Conference Location: Boston Marriott Copley Place
Paper Title: Subriemannian geodesics for coupled nonholonomic integrators
Authors: Eric W. Justh, P. S. Krishnaprasad
Acknowledged Federal Support: Y

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Publication Type: Conference Paper or Presentation **Publication Status:** 1-Published
Conference Name: 2018 IEEE Conference on Decision and Control (CDC)
Date Received: 19-Feb-2020 Conference Date: 17-Dec-2018 Date Published:
Conference Location: Miami Beach, FL
Paper Title: A variational problem on the probability simplex
Authors: Vidya Raju, P. S. Krishnaprasad
Acknowledged Federal Support: Y

DISSERTATIONS:

Publication Type: Thesis or Dissertation
Institution: UNIVERSITY OF CALIFORNIA DAVIS
Date Received: 29-Aug-2016 Completion Date: 6/16/16 5:57PM
Title: Mechanisms within the Black Box: Prediction, Computation, Randomness, and Complexity of Input-Output Processes via the γ -Transducer
Authors: NIX BARNETT
Acknowledged Federal Support: Y

Publication Type: Thesis or Dissertation
Institution: University of Maryland College Park
Date Received: 30-Aug-2017 Completion Date: 8/30/17 7:00AM
Title: Optimal Control of Heat Engines in Nonequilibrium Statistical Mechanics
Authors: Yunlong, Huang
Acknowledged Federal Support: Y

Publication Type: Thesis or Dissertation
Institution: University of California at Davis
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Authors: Paul Riechers
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Publication Type: Thesis or Dissertation
Institution: University of California at Davis
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Title: Exact Results Regarding the Physics of Complex Systems via Linear Algebra, Hidden Markov Models, and Information Theory
Authors: Paul Riechers
Acknowledged Federal Support: Y

Publication Type: Thesis or Dissertation
Institution: University of California, Davis
Date Received: 18-Aug-2018 Completion Date: 12/15/17 8:00AM
Title: Thermodynamics of Correlations and Structure in Information Engines
Authors: Alexander B. Boyd
Acknowledged Federal Support: Y

WEBSITES:

RPPR Final Report
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URL: <http://informationengines.org/>

Date Received: 31-Aug-2017

Title: Information Engines

Description: This is the website for the ARO MURI Information Engines: Nanoscale Control, Computing, and Communication Out of Equilibrium (W911NF-13-1-0390, 63822EGMUR).

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Description: Information Engine MURI project website

Final Report
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Information Engines:
Nanoscale Control, Computing, and Communication
Out of Equilibrium

Reporting Period: 1 September 2013 – 31 August 2020
ARO FY2013 MURI Topic #6
Transforming Information within Nonequilibrium Nanosystems
Topic Chief: Samuel C. Stanton

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Michael Roukes, California Institute of Technology (2017-2020)

Submitted to
<https://extranet.aro.army.mil>

Per online length limits, abridged versions were uploaded of the following Major Goals, Major Accomplishments, Training, Results Dissemination, Plans, Honors, and Tech Transfer. This document provides the detailed information from which the summaries in the main sections were derived and the abridged uploaded versions extracted.

NOTE: Despite solicitations for additional funds to continue research under the Information Engines MURI during its last (seventh) year (August 2019 – 2020), no funds were forthcoming. Thus, the most recent Interim Progress Report filed on 31 August 2019 and this Final Report cover only work up to 31 July 2019. That said, this Final Report and associated filings update publication and personnel information current as of this 2020 filing.

Major Goals

The Information Engines MURI's original goal was to develop a unified framework for understanding, designing, and implementing micron-scale and nanoscale information-processing engines and to provide the scientific foundation for future nanoscale devices with groundbreaking capabilities. These ambitious goals were met and, in several cases, exceeded as attested by the project's marked productivity; see <http://informationengines.org> $\Rightarrow$ Research. These successes opened up a number of exciting future theoretical and experimental research avenues. The main efforts successfully developed methods to control nanoscale thermodynamic processes and, perhaps most importantly, culminated in successful detailed experimental tests and verifications of our theoretical results. That said, looking beyond this MURI, much remains to do and the core PI team continues to collaborate on and extend the Information Engines MURI's progress. Putting the accomplishments in broad perspective, let's briefly review the overall project goals.

Any given natural process can be viewed in two complementary and equally valid ways: First, as a "physical" system that is controlled by, manipulates, stores, and dissipates energy and, second, as a "dynamical" system that generates, stores, transforms, and destroys information. When considering it and its physical implementation as a unitary system, we see that information processing requires energy to drive it forward. An immediate result is that this energy is not completely transformed into processed information. Energy is dissipated. Such limitations dominate on the nanoscale, in particular, where fluctuations out of equilibrium are the rule and the distinction between organized and thermal energy, between heat and work, becomes ambiguous. The MURI's principle goal, therefore, was to find the physical limits of nanoscale information processing and control.

To this end, the MURI pursued a set of interdependent tasks:

Task 1: *Intrinsic Computation in Nanoscale Substrates*: Develop concepts and mathematical tools that identify how dynamical processes store and transform information.

Task 2: *Nonequilibrium Information Processing by Nanoscale Machines*: Develop thermodynamic and statistical mechanical principles that govern the operation of information engines and then synthesize these with the tools of intrinsic computation from Task 1.

Task 3: *Control and Optimization at the Nanoscale*: Integrate methods of geometric optimal control theory and nonequilibrium statistical physics, instantiating the synthesis in concrete control problems posed by information engines.

Task 4: Validation: Optimal, Controllable Nanoscale Information Processing Agents: Develop experimental platforms with which to test the information-engines thermodynamic principles developed in Tasks 1, 2, and 3. These came to include nanoelectromechanical systems (NEMS) and flux qubits.

The ultimate experimental goal in Task 4 was to fabricate nanoscale devices capable of storing, manipulating, and retrieving information, as well as exploiting information as an energy-catalyst to generate motion and to direct the flow of energy. The allied theoretical challenges were to lay the scientific and engineering foundations for a new generation of denser, faster, cheaper, and more energy-efficient computing device capable of manipulating large-scale, complex data structures and to point the way to a new generation of self-organizing nanoscale engines capable collectively interfacing with the physical world with maximum power and efficiency.

The long-term scientific challenges, implicit in Tasks 1 – 3, were not only to pioneer theoretical foundations, but to also establish a research community in information engines. Looking back over the MURI's seven-year extended existence, there are two notable accomplishments on this score. The first is the annual workshop series on *Information Engines at the Frontiers of Nonequilibrium Thermodynamics*, co-organized by the Lead PI, held each summer at the Telluride Science Research Center, and sponsored by ARO; except in 2020 due to the pandemic. In lieu of an in-person workshop the co-organizers and past participants are assembling a special issue on *Thermodynamic Computing with Information Engines* for the well-known Journal of Statistical Physics.

The second is that the MURI's successes catalyzed the emergence of information engines as signaling the dawn of a new era of *thermodynamic computing* or, as we have come to frame it, *low- $k_B T$ computing*. The initial experimental successes and rapidly-progressing theory led the *Computing Community Consortium* (CCC) in January 2019 to initiate a broad planning effort to develop this new paradigm—whose charge is to actively leverage and control inherent fluctuations in physical information-processing substrates (<https://cra.org/ccc/events/thermodynamiccomputing/>). Note that in the 1990s and 2000s CCC was a key convener for research in quantum computing, among many other nascent information technologies. The current CCC effort is destined to play a similar guiding role for thermodynamic computing. Its report on *Thermodynamic Computing* is found at <https://arxiv.org/abs/1911.01968> and is uploaded with this Final Report. For those interested in delving further beyond this Final Report, we strongly recommend the CCC report as it paints a broad and bold picture of the path forward from this MURI.

Synopsis of Goals

NOTE: The MURI's annual Interim Progress Reports, filed each August, give detailed synopses of each year's goals. Here, limited space means that we can provide only the shortest summary of highlights. See also, the uploaded Final Report, which is not constrained by space.

The Information Engines MURI's led to major advances in controlling nanoscale thermodynamic systems and in determining the thermodynamic constraints on nanoscale information processing. In parallel, the MURI's flux-qubit information-engine devices were

calibrated and extensively experimented on. The experimental results successfully validated key aspects of our theoretical predictions and led to new theoretical advances—e.g., the *trajectory-class fluctuation theorems*. The flux-qubit device was demonstrated to be markedly more appropriate for the project’s goals than either the original molecular motor and NEMS systems. And so, it became our primary experimental platform. As a broad-brush summary, the following highlights our results in thermodynamic control, principles of information thermodynamics, and nanoscale information-engines experiments.

A. Control of Nanoscale Thermodynamic Systems: Bringing together methods of geometric optimal control theory and nonequilibrium statistical physics, instantiated in concrete problems of designing working cycles for heat engines, has been a major goal of this part of the MURI project. The UCD-UMD teams focused on one of our three previously-developed approaches to controlling nanoscale thermodynamics systems: counterdiabatic control protocols for information processing tasks. Addressing very practical trade-offs in computing, counterdiabatic protocols provide finite-time “short-cuts” to, what otherwise are, adiabatic control protocols that require infinite time. PIs Crutchfield and Jarzynski continued to synthesize this control approach with the geometric and engineering control theories by analyzing all of the elementary bit manipulations (erase, create, swap, invert, and the like).

An additional goal for UMD (PI Krishnaprasad) was to make progress in collective dynamics (theory and data analysis) to incorporate symmetry, geometry, and information propagation through wave phenomena, learning, and the influence of noise. (Of particular interest was the subject of sub-Riemannian geometry, primarily as a tool for achieving these goals.)

B. Principles of Information Thermodynamics: UCD determined the costs of thermodynamic controller’s modular organization—the *modularity dissipation*—the first time thermodynamic costs have been associated with a system’s structure and organization. This advances our suite of theoretical results to a design methodology for nanoscale devices with net positive thermodynamic benefit. And, critically, it laid the foundation (See Table I in the CCC report) for an extensive suite of experimental tests that continue on under other projects.

C. Nanoscale Information Engines Experiments: Due to key theoretical insights, the flux qubit became the main experimental focus. In the process, UCD-Caltech discovered new ways—called the trajectory-class fluctuation theorems—to diagnose success and failure modes of microscopic behaviors that support information processing using the mesoscopic “observable” of the distribution of works expended over a repeated protocol. That is, the flux-qubit experiments demonstrated how a relatively-accessible thermodynamic observable (work) could be used to diagnose the success and failure of microscopic information processing trajectories. We proved that work distributions obey their own, characteristic Jarzynski integral and Crooks detailed fluctuation theorems and that the trajectory-class fluctuation theorems synthesize them both in a single family.

Critically, the experiments demonstrated that flux qubits offer a number of benefits for information-engine experimentation in terms of controllability, reliability, and speed of operation. These are particularly important when validating fluctuation theorems, as the latter require sampling extremely rare events and so many millions of experimental repetitions.

Finally, two experimental thermodynamic-measurement technologies were designed. For near-term experimentation this included bolometric measurements for acquiring average thermodynamic quantities using electron heat baths in normal metal islands. For the longer-term, this included calorimetric measurements for acquiring distributions of thermodynamic quantities in semiconducting islands using one-shot protocols. Preliminary data on normal metal islands showed that the required sensitivity to make averaged measurements is attainable with next-round fabrication. First-round fabrication and testing of semiconductor platforms was completed. Moving forward to implement these experiments only relies on the PIs' ability to attract financial support, since this MURI established the necessary experimental infrastructure.

Overall, the MURI was remarkably productive with well over 100 peer-reviewed published articles:

2019: Thirty-eight manuscripts were in play: 19 appearing in peer-reviewed, high-profile journals, another 11 manuscripts under review, and 8 in preparation.

2018: Over 40 manuscripts were in play: 25 appearing in peer-reviewed, high-profile journals, another 11 manuscripts under review, and 4 in preparation.

2017: Over 52 manuscripts: 35 appearing in peer-reviewed, high-profile journals and another 17 manuscripts under review.

2016: Over 40 manuscripts: 24 appearing in peer-reviewed, high-profile journals and another 21 manuscripts submitted.

Most all are available through arXiv.org and the project website: <http://informationengines.org>. Importantly, 13 appeared in physics' top journals: 6 in *Physical Review X* and 7 in *Physical Review Letters*. Thus, the MURI's efforts were recognized at the highest levels and had substantial impact. Moreover, the high productivity and substantive results reflect a project-wide technical maturation and the close collaborations across the MURI teams. The statistics reveal that the MURI's previous years' exceptional productivity was sustained each year. Practically speaking, the MURI teams made good on all of the original proposal's four Tasks, excepting the early emphasis on molecular motors.

Administratively, the Information Engines MURI (#W911NF-18-1-0340) complements the Lead PI's ARO project *Functional Pattern Formation in Thermodynamical Systems* (#W911NF-18-1-0028). The latter started in 2018 and focuses on spatially-extended engines with the unique goal of tracking the flow of thermodynamic resources. In contrast, the MURI itself concerned individual engines and provided a wealth of new tools for analyzing spatially-distributed information engines. The two projects' conceptual and, even, algorithmic commonalities translated into quite of bit of conceptual exchange and synergistic progress.

Accomplished under Goals

The following reviews the PIs' efforts in turn. (Citation [XXX#] are listed in the Bibliography.)

PI Crooks: Continued his signature geometric approach to thermodynamic control and also contributed fundamental theoretical work on strongly coupled thermodynamic subsystems.

1. **Thermodynamic geometry of minimum dissipation driven barrier crossing** [GEC1]: Explored the thermodynamic geometry of a simple system that models the bistable dynamics of nucleic acid hairpins in single molecule force-extension experiments. The analysis demonstrated that the friction coefficient of the driving protocols is sharply peaked at the interface between metastable regions, which leads to minimum-dissipation protocols that drive rapidly within a metastable basin, but then linger longest at the interface, giving thermal fluctuations maximal time to kick the system over the barrier. This provides a design principle for constructing thermodynamically efficient coupling between stochastic objects and predicts key aspects of evolved biomolecular motors.
2. **Near optimal protocols in complex nonequilibrium transformations** [GEC2]: Crooks described a general method for sampling an ensemble of finite-time, nonequilibrium protocols biased toward a low average dissipation. As an application, Crooks sampled the ensemble of low-dissipation protocols that invert the magnetization of a 2D Ising model and explored how the diversity of the protocols varies in response to constraints on the average dissipation.
3. **Geometric approach to optimal nonequilibrium control** [GEC3]: Optimal control of nanomagnets has become an urgent problem for the field of spintronics as technological tools approach thermodynamically determined limits of efficiency. Crooks provided a physically transparent derivation of a metric tensor for which the length of a protocol is proportional to its dissipation. Crooks then described a numerical method that computes geodesics even when the number of control parameters is large. Crooks' calculations revealed nontrivial protocols for magnetic-spin bit erasure and reversal, providing important, experimentally testable predictions for ultra-low-power computing.

PI Crooks left the MURI Project during 2017 to develop a start-up company developing quantum machine learning.

PI Crutchfield: Despite a number of focused technical questions still to analyze, computational mechanics' account of information processing embedded in thermodynamic systems is close to complete. In short, it can explain and analyze a broad array of thermodynamic information processing with mathematical and numerical precision. For example, Crutchfield developed the trajectory-class fluctuation theorems, synthesizing those of Jarzynski and Crooks, to delineate how engines function and fail on a given informational task. And, there is a new level of exact analysis of information engine operation that can be used to identify their possible thermodynamic functioning and how those functions fluctuate on the nanoscale. Here's brief summary that gives a sense of the depth and breadth of results:

- **Functional fluctuations** [JPC1]: Large deviation theory and computational mechanics predict how the thermodynamic functioning of information engines fluctuates in response to environmental behaviors. Previous conjectures have been rigorously established and the

manuscript appropriately updated.

- **Costs of modularity** [JPC3]: Perhaps the most surprising and broadly applicable result to come out of the thermodynamic analysis of intrinsic computation is that the modular architecture of an information engine comes at a thermodynamic cost. In short, modularly-organized systems require more input work to run and they dissipate more energy in their operation. This goes far beyond Landauer's original argument, that only erasure of information implied a thermodynamic cost, to demonstrate that the very modular organization of information processing devices, whether digital circuits or biological organisms, extracts a thermodynamic cost. In short, inefficiency arises from modularity by destroying the ability to leverage environmental correlations.
- **Powerful mathematical and calculation methods** [JPC5]: Many results rely on our introducing wholly new mathematical tools. Without these, most results described here and their future generalizations would not be accessible. Moreover, the new methods are sufficiently powerful to yield closed-form analyses in many previously-intractable cases.
- **Computational mechanics of infinite-memory processes** [JPC6]: Many systems of interest in stochastic thermodynamics have continuous state spaces. Availing ourselves of the mathematical properties of computational mechanics' causal states led to our extending the analysis of intrinsic computation to such infinite-state systems. This opens up a vast array of future applications. The molecular sensors analyzed are just a first example.
- **Multivariate mutual information** [JPC7,JPC16,JPC18]: Computational mechanics' analysis of intrinsic computation relies critically on tools and concepts from information theory. As such, Crutchfield maintains an active research thrust in developing various kinds of information measures and algorithms to estimate them. For example, after calling into question many of the uses of mutual information to diagnose complex systems, he finally introduced a constructive approach for this important task. A key step in detecting that an information engine has formed patterns relies on using mutual information shared across a field of random variables. New information-theoretic methods were developed to handle this case. A comprehensive software package in Python was developed and is available as open source.
- **Toward quantum information engines** [JPC8]: With an eye to future directions for information engines, Crutchfield explored the structural complexity in quantum processes. The results suggest that quantum information engines will exhibit a surprising array of new thermodynamic behaviors. In particular, quantum models of stochastic processes can be smaller than classical. In contrast with the ϵ -machine's unique role in the classical setting, however, among the class of processes described by pure-state hidden quantum Markov models, there are those for which there does not exist any strongly minimal model. This hints at a fundamental ambiguity between classical and quantum physics.
- **The Principles of Requisite Complexity** [JPC10]: For an adaptive system to take maximum thermodynamic advantage of its environment, it must be internally organized to represent its environment's correlations.
- **Bacteria as environmental prediction engines** [JPC11]: Crutchfield developed a novel application of computational mechanics and information engines that explains the role of bacterial epigenetics as coding predictive ("causal") states of the environment.
- **Causal asymmetry in a quantum world** [JPC12]: Over two decades ago PI Crutchfield discovered the structural asymmetry in stationary processes "played" in forward and reverse time. It turns out that this is a classical phenomenon, as the quantum structural complexity is

time symmetric. This raises fundamental issues about the origins of asymmetry in classical physics and so in thermodynamic information processing.

- **Spacetime computational mechanics** [JPC13]: Although the possibility and formal constructions of computational mechanics for spatially extended systems has been known for three decades, it has been left largely unexplored. This effort laid out the theoretical foundations for structure and causality in spacetime, drawing connections with invariant-set theory of dynamical systems.
- **Information theory software package** [JPC17]: Crutchfield published an open source Python library for discrete information theory.
- **Fraudulent white noise** [JPC18]: Crutchfield gave a new view of “unstructured” and “uncorrelated” processes that goes some distance to disabuse us of misinterpreting or even simply dismissing structure present in apparently-noisy observations.
- **Information engine performance** [JPC19]: Crutchfield developed new error-dissipation trade-offs in information engines controlled via time-symmetric protocols.
- **Measurement-induced randomness and structure** [JPC20]: Measurement is a crucial act in both classical nonlinear dynamics and in quantum dynamics. Crutchfield developed close parallels and distinctions between quantum and classical physics in terms of randomness and structure that measurement can generate or remove.
- **Harnessing fluctuations in thermodynamic computing** [JPC21]: Crutchfield developed mesoscopic methods to track successful and failed microscopic information processing. This is a key step to adapting fluctuation theorems to spatially-extended information engines. This new approach was experimentally validated.
- **Shortcuts to thermodynamic computing** [JPC22]: Spatially-extended information engines present a particularly challenging spatiotemporal control problem. Crutchfield and Jarzynski developed new counterdiabatic control methods that give much advantage in this case.

PI DeWeese: Developed new approaches for understanding and controlling nonequilibrium systems and applied these insights to network theory, learning, engineered systems, and fundamental physics problems.

Geometric control and learning: DeWeese generalized the geometric framework for finding minimum dissipation protocols to include a systematic expansion of all terms beyond the second-order equations known previously, as well as a generalization of the “escorted dynamics” framework for transitioning the full distribution of a thermodynamic system from one state to another in finite time to the case of more than one control parameter. This included developing a technique to identify critical points in the loss surfaces explored during learning in dynamical systems far from equilibrium [MRD1], a study comparing and contrasting the sparse structures of natural scenes versus natural sounds viewed as nonequilibrium physical systems [MRD2], and an analysis of fault tolerance in the design of optical neural networks that depend on various types of nonlinearities to overcome thermal fluctuations that limit performance [MRD3].

PI Jarzynski: Continued to pioneer novel control strategies for classical and quantum thermodynamic systems.

Thermodynamics of periodically-driven systems: When a stochastic system is perturbed by external, time-periodic forcing, it reaches a periodic state, characterized by currents and entropy production that are analogous to those that arise in nonequilibrium steady states. Earlier work

funded by the MURI showed for discrete-state Markov dynamics that such *stochastic pumps*—periodically driven stochastic systems—are able to mimic nonequilibrium steady states, achieving the same time-averaged currents and probabilities at the same thermodynamic cost of entropy production [CJ5]. Jarzynski recently extended this to diffusive motion in one degree of freedom [CJ1]. In contrast to the discrete-state case, Jarzynski found that for a given average current and probability distribution, a periodically-driven diffusive system always generates more entropy than a nonequilibrium steady state (NESS). Additionally, Jarzynski showed how to construct both a stochastic pump and a NESS that support a given, desired current and probability distribution.

Programmable Maxwell’s Demon: Jarzynski developed a mechanistic model of a *programmable* Maxwell’s Demon [CJ2], which interacts with a thermal bath, a mass that can be lifted against gravity, and a sequence of *bits* implemented by paddles that rotate around a central axle. The model is programmable in the sense that it can be designed so that if the arriving bits encode a particular sequence—say the binary representation of $\pi=3.14159\dots$ —then the device extracts energy from the reservoir and delivers it to lift the mass. Conversely, if the mass is very large then the device systematically writes the digits of π onto the stream of bits, at a thermodynamic cost equal to that predicted for bit erasure by Landauer’s principle. Jarzynski provided exact solutions for the behavior of the device in a particular limit and showed that our model can realize both autonomous and nonautonomous versions of Maxwell’s demon.

Second Law violations: One of the major themes explored over the MURI is that, for sufficiently small systems, fluctuations give rise to occasional “violations” of the Second Law of thermodynamics. In particular, for isothermal processes the Second Law inequality $W \geq \Delta F$ need not be satisfied for every realization of a given process, as long as it is satisfied on average. Jarzynski explored whether universal bounds can be placed on the probability to observe such violations of the Second Law and showed that it is possible, in principle, to design protocols in which most realizations give rise to Second Law violations, but the inequality remains satisfied on average. Such protocols have recently been implemented experimentally using a single-electron transistor [CJ3].

Shortcuts to adiabaticity: These are control strategies for achieving adiabatic evolution under nonadiabatic (fast) driving. A major focus of Jarzynski’s research efforts developed methods to construct shortcuts for a variety of systems—classical, quantum and stochastic—thereby providing a robust and broadly applicable set of tools for controlling systems of interest. Earlier work funded by this MURI showed that a broad range of shortcuts to adiabaticity that can be unified within a single theoretical framework using *flow fields*, providing both intuition and a roadmap for further progress [CJ6].

Counterdiabatic erasure: Crutchfield and Jarzynski applied this approach to the problem of bit erasure, in which an overdamped Brownian particle evolves in a double-well potential and the aim is to design a protocol that rapidly forces the particle into one of the wells [JPC22]. Crutchfield and Jarzynski derived an exact expression for the additional work required to implement this protocol and clarified how this work scales with the protocol duration, the system size, and the implemented information processing. This project ties together a number of strands investigated over the course of the MURI: thermodynamics of information processing, geometric control, and shortcuts to adiabaticity.

Quantum adiabatic control: For quantum systems, we constructed local shortcuts to adiabaticity that rapidly drive a system from an excited state of an initial Hamiltonian to the

corresponding state of the final Hamiltonian [CJ4]. This result solves an important open problem in the field, as previously local quantum shortcuts were available only for the ground state. Our strategy combines the flow field method mentioned above with a semiclassical analysis.

Periodically-driven Hamiltonian control: More recently, Jarzynski applied our flow field method to classical, Hamiltonian systems that are driven periodically with time. We showed how to construct a time-periodic potential that suppresses all excitations above a chosen value of energy, and we are currently exploring the quantum version of this problem.

Impulse-control of Hamiltonian dynamics: Finally, in the course of developing quantum shortcuts to adiabaticity, Jarzynski introduced a class of Hermitian operators that act as generators of spatial deformations. Jarzynski recently applied these operators to explore how quantum systems can be controlled by the application of impulses—i.e., infinitely strong and infinitesimally brief perturbations. He found that such perturbations are naturally divided into first-order and second-order impulses, and we solved exactly for their effects.

PI Krishnaprasad: Developed approaches to control nonequilibrium processes, applying them to thermodynamic computation, collective motion, population dynamics, and interface growth.

Thermodynamic efficiency in a stochastic dissipative oscillator [PSK1]: A significant breakthrough was made in formulating and solving the design problem of a cyclic protocol (heat engine) that extracts a prescribed amount of work with maximal thermodynamic efficiency in a stochastic dissipative system (model problem: an oscillator coupled to a heat bath). The overdamped version (exemplified by a controllable capacitor in contact with a Nyquist-Johnson resistor in a heat bath of controllable temperature) is technically more complex and is being prepared for publication.

Subriemannian geometry in collective motion [PSK3,PSK4,PSK5]: Previous work on collective subriemannian geometry was further extended to continuum settings with a view towards understanding long-range propagation of information in collectives. Further development that incorporates stochasticity in collectives is expected.

Population games and their control [PSK2,PSK4,PSK7]: Significant progress was made in the area of population games and their control. Specifically, this took the form of investigating a variational principle for replicator dynamics on the probability simplex and new controllability results for such games when the associated payoff/fitness maps are modulated.

Controlling KPZ interface growth [PSK6]: Krishnaprasad made progress on control of the KPZ equation of interface growth, specifically to solve the variance minimization problem on a finite-time horizon.

PI Roukes: Roukes' Caltech team demonstrated that superconducting flux qubits can act as nanoscale switches displaying strong fluctuations at low temperatures. In particular, the flux qubits were validated as ideal classical double-well systems at temperatures near 500 mK. In collaboration with the UC Davis team, functional partitions within an erasure protocol were experimentally verified using the flux qubit [JPC21,MR1]. To monitor the thermodynamics, Caltech measured thermal conductance of suspended superconducting-normal-superconducting (SNS) thermometers and found a strong reduction of thermal conductance necessary for the thermodynamic measurements of information processing in flux qubits. Combining the SNS junction thermometers with the flux qubits on the same chip is underway in collaboration with Siyuan Han (University of Kansas). Roukes' Caltech team designed the flux qubit/SNS thermometer chip and reconfiguring the measurement equipment for thermodynamic

measurements of operations within the flux qubit. It also completed first-round fabrication of novel Superconductor-Semiconductor-Superconductor (S-Sm-S) junctions and Superconductor-Graphene-Superconductor (S-Gr-S) junctions for single-shot calorimetric detection of nanoscale information processes, in collaboration with the Palmstrom group (UCSB) and Nadj-Perge group (Caltech), respectively.

PI Hess: Explored how velocity fluctuations in microtubule transport by surface-adhered kinesin motors revealed key insights on how the degree of velocity fluctuations directly relates to a loss in efficiency and on how heterogeneity in motor attachment geometry and the anharmonicity in the tail stiffness conspire to dominate the velocity fluctuations at high motor densities. The experimental data led him to explore bounds on the entropy production rate as a function of the positional uncertainty. Second, Hess also initiated a detailed analysis of the information thermodynamics of the kinesin step to determine which fraction of the energy dissipated by kinesin is lost due to information processing. Finally, his work also investigated self-assembling, force-producing structures. His Columbia University team left the MURI project during Fall 2016.

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- [PSK4] V. Raju and P. S. Krishnaprasad “Lie Algebra Structure of Fitness, and Replicator Control,” 23 pages, **under review**.
- [PSK5] U. Halder, V. Raju, et. al. “Cognitive Cost of Flocking: A Geometric and Hamiltonian Perspective,” 21 pages, **under review**.
- [PSK6] Y. Huang and P. S. Krishnaprasad (2018) “Optimal Control of KPZ Equation using Deep Reinforcement Learning”, 11 pages; **under review**.
- [PSK7] U. Halder, Eric W. Justh and P. S. Krishnaprasad, “Continuum Flocking and Control,” 23 pages, **under review**.
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Training

The Information Engine MURI training effort was substantial with an average of half a dozen postdoctoral and two dozen graduate researchers, with 20 PhDs granted.

2019: 7 postdoctoral researchers, 18 graduate student researchers, and an undergraduate research intern. Five PhD degrees.

2018: 8 postdoctoral researchers, 20 graduate student researchers, and several undergraduate research interns. Three PhD degrees.

2017: 7 postdoctoral researchers, 20 graduate student researchers, and several undergraduate research interns. Six PhD degrees.

2016: 7 postdoctoral researchers, 29 graduate student researchers, and several undergraduate research interns. Five PhD degrees, one MS degree.

Ph.D. Degrees Earned

- Cina Aghamohammadi: “Memory and Thermodynamic Costs of Sampling and Biased Sampling”, Ph.D. Dissertation in Physics, University of California at Davis, August 2018.
- Mayur Mudigonda, “Inference algorithms and sensorimotor representations in brains and machines”, PhD dissertation in Vision Science, University of California at Berkeley, June 2019.
- Udit Halder: “Optimality, Synthesis and a Continuum Model for Collective Motion”, Ph.D. in Engineering, University of Maryland, College Park, April 2019.
- Vidya Radu: “Collective Behavior, Information Propagation, and Noise”, Ph.D. in Engineering, University of Maryland, College Park, May 2019.
- Eric Dodds: “Statistical learning models of sensory processing and implications of biological constraints”, PhD dissertation in Physics, December 2018.
- Alexander Boyd: “Thermodynamics of Correlations and Structure in Information Engines”, Ph.D. Dissertation in Physics, University of California at Davis, December 2017.
- Ayoti Patra, “Bridging quantum, classical and stochastic shortcuts to adiabaticity”, PhD in Physics, University of Maryland, College Park, September 2017.
- Y. Huang: “Optimal control of heat engines in non-equilibrium statistical mechanics”, PhD in Engineering; August 2017.
- Nix Barnett: “Mechanisms within the Black Box: Prediction, Computation, Randomness, and Complexity of Input-Output Processes via the ε -Transducer”, PhD in Mathematics, University of California, Davis, August 2016.
- Sarah E. Marzen: “Bio-inspired Problems in Rate-distortion Theory”, PhD in Physics, University of California, Berkeley, August 2016. Now, Physics of Living System Fellow with Prof. Jeremy England, Physics, MIT.
- Paul Riechers: “Exact Results Regarding the Physics of Complex Systems via Linear Algebra, Hidden Markov Models, and Information Theory”, Ph.D. Dissertation in Physics, University of California at Davis, December 2016.
- J. Demers, “Stochastic processes in physics: deterministic origins and controls”, PhD in Physics, University of Maryland, College Park, December 2016. Dr. Demers is now a postdoc in Prof. William Fagan’s group in the Department of Biology, University of Maryland, College Park.

- Amy T-C. Lam, “Assembly in Dynamic Nanoscale Systems”, PhD in Biomedical Engineering, Columbia University, New York, December 2015.
- Zhiyue Lu: “Topics in equilibrium and nonequilibrium thermodynamics: computing crystalline free energies and engineering Maxwell’s demon”, PhD in Chemical Physics, University of Maryland, College Park, December 2015.
- Biswadip Dey (UMD, 2014); Now, Postdoctoral Fellow in Mech & Aero Eng, Princeton University.
- Patrick Zulkowski (UCB, 2014) “The Geometry of Thermodynamic Control”; Now, Assistant Professor, Berkeley City College.
- Ofer Idan (Columbia, 2014) “Modeling Nanoscale Transport Systems”.
- Nick Travers (UCD, 2014); Now, Asst. Prof, Mathematics, University of Indiana, Bloomington.
- Ryan G. James (Physics, UC Davis) Ph.D. August 2013.
- Nicholas F. Travers (Mathematics, UC Davis) Ph.D. August 2013.

M.S. Degrees Earned During Reporting Period

- K. Miltenberger, MS thesis on collective behavior. April 2016.

Additional information on programs, students, and faculty of the Information Engines MURI project and the Complexity Sciences Center is available online at <http://informationengines.org/> and <http://csc.ucdavis.edu/>, respectively.

The list of trainees—postdoctoral, graduate, and undergraduate students—follows. (0% FTE means a researcher substantially participated in advancing project goals, but did not receive direct financial support from the project.)

Research Scientists Involved

- Warren Fon (Physics, Caltech) 20% FTE.
- Matthew Matheny (Physics, Caltech) 50% FTE.
- Korana Burke (Lecturer in Mathematics, UC Davis).
- John Mahoney (Lecturer in Mathematics, UC Davis).
- Dowman Varn (Lecturer in Mathematics, UC Davis).

Postdoctoral Researchers Involved

- Fabio Anza (Physics, UCD) TWCF Fellow, 0% FTE.
- Alec Boyd (Center for Quantum Technologies, U. Singapore), TWCF Fellow, 0% FTE.
- Korana Burke (Physics, UCD) September 2012-2015, UC Davis Chancellor’s Postdoctoral Fellowship. 0% FTE.
- Ryan James (Physics, UCD) 10% FTE.
- Sarah Marzen (Physics, MIT) Physics of Life Fellowship, 0% FTE.
- Paul Riechers (Center for Quantum Technologies, U. Singapore), 0% FTE.
- Olli-Pentti Saira (Physics, Caltech) 100% FTE.
- Cina Aghamohammadi (Woods Hole Oceanographic Institution), 0% FTE.
- Louis Kang (Physics, UCB) 0% FTE.
- Dibyendu Mandal (Physics, UCB) 100% FTE.
- Jascha Sohl-Dickstein (Google; Neuroscience, Stanford) 0% FTE.

- John Mahoney (Physics, UCD) 0% FTE.
- Parag Katira, Ph.D. (Associate Research Scientist, Columbia), 50% FTE.
- Patrick Zulkowski (Physics, UCB) 25% FTE.
- Sebastian Deffner (Chemical Physics, Maryland), 100% from 9/2013-8/2014; 100% FTE.

Graduate Students Involved

- Jeff Emenheiser (Physics, UCD), Ph.D. candidate. 0% FTE.
- David Gier (Physics, UCD), Ph.D. candidate. NSF Graduate Fellow. 0% FTE.
- Wade Hodson (Physics, UMD), Ph.D. candidate. 50% FTE.
- Xincheng Li (Engineering, UMD), Ph.D. candidate. 100% FTE.
- Alexandra Jurgens (Physics, UCD), Ph.D. candidate. 20% FTE.
- Raj Katti (Physics, CalTech), PhD candidate. 20% FTE.
- Xincheng Lei (Physics, UCD), Ph.D. candidate. 50% FTE.
- Sam Loomis (Physics, UCD), Ph.D. candidate. 25% FTE.
- Dani Masante (Physics, UCD), Ph.D. candidate, UCMEXUS Graduate Fellow. 0% FTE.
- Adam Rupe (Physics, UCD), Ph.D. student. 25% FTE.
- Pratik Sachdeva (Chemistry, UCB), Ph.D. student. 0% FTE.
- Ariadna Venegas-Li (Physics, UCD), Ph.D. candidate. 20% FTE.
- Kyle Ray (Physics, UCD), Ph.D. candidate. 50% FTE.
- Neha Wadia (Physics, UCB), Ph.D. student. 0% FTE.
- Greg Wimsatt (Physics, UCD), Ph.D. candidate. 100% FTE.
- Ryan Zarcone (Physics, UCB), Ph.D. student. 0% FTE.
- Michael Fang (Physics, UCB), Ph.D. student. 0% FTE.
- Andrew Ligeralde (Physics, UCB), Ph.D. student. 0% FTE.
- Charles Frye (Physics, UCB), Ph.D. student. 0% FTE.
- Steven Lee (Physics, UCB), Ph.D. student. 0% FTE.
- Mayur Mudigonda (Physics, UCB), Ph.D. student. 0% FTE.
- Tyler Maltba (Physics, UCB), Ph.D. student. 0% FTE.
- Nick CinkoAdam Frim (Physics, UCB), Ph.D. student. 0% FTE.
- Cina Aghamohammadi (Physics, UCD), Ph.D. student. 47% FTE.
- Alec Boyd (Physics, UCD), PhD candidate. 47% FTE.
- Eric Dodds (Physics, UCB), Ph.D. student. 0% FTE.
- Udit Halder (Engineering, UMD) Ph.D. candidate. 0% FTE. Ph.D. Expected April 2019: collective behavior, information propagation and noise.
- Yunlong Huang (Engineering, UMD) Ph.D. August 2017. 100% FTE.
- Katherine Klymko (Chemistry, UCB), Ph.D. student. 0% FTE.
- Vidya Radu (Engineering, UMD) Ph.D. candidate. 50% FTE. Expected April 2019: collective behavior, replicator dynamics and control, and noise.
- Andrew Mavin Smith (Chemical Physics, Maryland), PhD candidate. 50% FTE.
- Joseph Demers (Chemical Physics, Maryland), PhD candidate. 50% FTE.
- Nix Barnett (Mathematics, UCD), PhD candidate. 47% FTE.
- Paul Riechers (Physics, UCD), PhD candidate. 47% FTE.
- Dmitry Shemetov (Mathematics, UCD), Ph.D. student. 0% FTE.
- Henri Palacci (Biomedical Eng., Columbia), PhD candidate. 50% FTE.
- V. Raju (Engineering, UMD) Ph.D. 0% FTE.
- Michael Prijatelj (Physics, CalTech), Ph.D. Candidate. 0% FTE.

- Megan Armstrong (Biomedical Eng., Columbia), PhD candidate. 12% FTE.
- Ofer Idan (Biomedical Eng., Columbia), PhD candidate. 18% FTE.
- Amy Lam (Biomedical Eng., Columbia), PhD candidate. 17% FTE.
- Ayoti Patri (Chemical Physics, Maryland), PhD candidate. 50% FTE.
- Zhiyue Lu (Chemical Physics, Maryland), PhD candidate. 50% FTE.
- Biswadip Dey (Elec. Comp. Eng., Maryland), PhD candidate. 0% FTE.
- Patrick R. Zulkowski, (Physics, UCB) Ph.D. August 2013. 50% FTE.
- Pooneh Ara (Physics, UCD), PhD candidate. 47% FTE (NetControl MURI).
- Benny Brown (Physics, UCD), Ph.D. candidate. 0% FTE.
- Sarah Marzen (Physics, UCB), Ph.D. student. UC Berkeley & NSF Fellowships. 0% FTE.
- Grant Rotskoff (Chemistry, UCB), Ph.D. candidate. 0% FTE.
- K. Miltenberger (Elec. Comp. Eng., GSR) 50% FTE.
- Neda Bassir Kazeruni (Biomedical Eng., Columbia), PhD candidate. 17% FTE.
- Stanislav Tsitkov (Biomedical Eng., Columbia), PhD candidate. 16% FTE.

Undergraduate Students Involved

- Sara Pohland Huang (Engineering, UMD), B.S. student. 0% FTE.
- Hyun Su Kim (NSF REU undergraduate intern, Physics, UCD, 2017) 0% FTE.
- Bahti Zakirov (NSF REU undergraduate intern, Physics, UCD, 2017) 0% FTE.
- Josh Ruebeck (NSF REU undergraduate intern, Physics, UCD, 2016) 0% FTE.
- Brent Schlotfeldt (Engineering, UMD, 2017), pursuing PhD study in Electrical Engineering at the University of Pennsylvania.
- David Gier (NSF REU undergraduate intern, Physics, UCD, 2015) 0% FTE.
- Alexandra Nilles (NSF REU undergraduate intern, Physics, UCD, 2014) 0% FTE.
- Andrew Berger (Physics, UCB, 2015) 0% FTE.
- Brendan Roberts (NSF REU undergraduate intern, Physics, UCD, 2013).
- Greg Wimsatt (Undergraduate intern, Physics, UCD).

Results Dissemination

The Information Engines MURI's productivity was sustained at a high level, indicating an intellectual maturation as the teams overcame previous theoretical and experimental challenges. The results were disseminated rather widely. Annual summary:

2019: Thirty-eight manuscripts were in play, 19 appeared in peer-reviewed, high-profile journals, another 11 manuscripts were under review, and 8 were in preparation.

2018: 40 manuscripts, 25 appeared in peer-reviewed, high-profile journals and another 11 manuscripts under review.

2017: 52 manuscripts, 35 appeared in peer-reviewed, high-profile journals and another 17 manuscripts were under review.

2016: 40 manuscripts, 24 appeared in peer-reviewed, high-profile journals and another 21 manuscripts were submitted.

Each year during the MURI, the Lead PI co-organized the workshop on *Information Engines at the Frontier of Nanoscale Thermodynamics*, held at the Telluride Science Research Center, typically 10 days during July, and supported by ARO. The Lead PI also organized *Beyond Shannon—The Structure and Meaning of Information*, held at the Institute for Advanced Study, University of Amsterdam, 6-8 May 2019.

Space does not permit listing the hundreds of presentations—team colloquia, keynotes, lecture courses, invited presentations, and team-organized meetings and workshops. These are, however, documented in detail in the annual Interim Progress Reports.

Plans

The MURI, active over seven years, two over the usual duration of five years, has ended. Much remains to do, of course, despite the its marked accomplishments. The team was graced with discovering powerful theoretical results and a state-of-the-art experimental platform on which to test them and to explore additional ideas. It will continue to use its meeting-workshops in Telluride to monitor the coming challenges and to follow-through on our current research foci.

Appreciating future challenges requires recalling that it underwent a substantial change in organization, pivoting to the flux qubit devices of the Roukes group at Caltech. Our second “volunteer” experimentalist, Jukka Pekola (Aalto University, Finland), actively collaborated with the team us on the challenges of designing devices for yoctojoule calorimetry and bolometry and for scaling up to coupled information engines.

Looking forward, beyond the MURI, several of the more specific plans the PIs will pursue are listed in the following.

PI Crutchfield: Our primary effort will merge our theoretical progress on the thermodynamics of information engines and information ratchets with the experimental realizations developed by the Caltech team. In fact, PI Crutchfield spent half a sabbatical year in the Roukes lab helping to drive this effort. Our theoretical efforts will also continue with foundational questions on the limits, trade-offs, and capabilities of information engines in terms of fluctuations and large deviations from thermodynamic functioning and also directly probing the thermodynamic costs of modularity. We are now actively designing information engines circuits and lattices and seeking financial support for these efforts.

PI Roukes: The team completed flux qubit thermodynamic experiments, extracting detailed data to validate the UC Davis fluctuation theorem predictions. This proved to be a rich system with many positive attributes for experiments on nanoscale information processing. We are continuing to pursue development of on-board bolometric thermodynamic measurements; a variety of structures based on both epitaxial Al/InAs and single-layer graphene were designed and fabricated. Additionally, we continue to advance our understanding of calorimetric measurements to detect quantum transitions through the local heat bath. Construction of prototype calorimeters using superconducting-semiconducting-superconducting (SNS) junctions to restrict the number of electron states to achieve very small energy resolutions is underway. Currently, the Roukes group in the process of having these junctions grown (via epitaxy) in collaboration with the Palmstrom group at UC Santa Barbara and the Nadj-Perge group at Caltech. Designs that are compatible with bolometric measurements of classical logic erasure are underway. There are only minor adjustments to the experimental platform to measure thermodynamic changes within quantum processes. Caltech plans on performing thermodynamic measurements of quantum processes immediately following measurements of the classical counterparts.

Honors, Awards, and Appointments

Space does not permit listing the dozens of PI honors, awards, and appointments. These are, however, documented in detail in the annual Interim Progress Reports.

Tech Transfer

- **PI Crutchfield:** Continues to maintain and augment the MURI's website <http://informationengines.org/> to facilitate team collaborations and outreach.
- **PI Crutchfield:** Continues to develop the open source Python package “Computational Mechanics in Python” (CMPy) consisting of most of computational mechanics’ constructive mathematical results and methods. Jupyter/Python notebooks continue to be developed to illustrate calculational details reported in our publications. A suite of over two-dozen Jupyter notebooks was developed as tutorials. CMPy has been ported to run on the Jupyter notebook service CoCalc.com. Efforts initiated to port CMPy from Python 2.7.X to Python 3.X.
- **PI Crutchfield:** Further developed the open source *Discrete Information Theory* Python package dit: <https://github.com/dit/dit>. Most notably, it was extended to include an even more complete suite of multivariate information measures for dynamical and stochastic networks. Including, in particular, new algorithms for secret key agreement measures of unique information [JPC17].
- **PI Krishnaprasad:** Transfer of knowledge to the Naval Research Laboratory through collaboration with Dr. Eric Justh has continued on a regular basis. Concrete applications of this transfer effort are expected in the area of collective behavior in unmanned aerial and marine systems. Other applications to development of machine learning algorithms are also under consideration.
- **PI Krishnaprasad:** There have been multiple interactions with Dr. Adam Svenkeson (Research Scientist at Army Research Laboratory, Aberdeen, MD) and these are expected to continue on a monthly basis, with the aim of developing collaborations.
- **PI Krishnaprasad:** Additional collaboration with Northrop Grumman Mission Systems (contact: Dr. Isidoros Doxas) has been initiated to allow further developments in the direction of adversarial learning modeled by controlled replicator dynamics subject to noise. Applications are being considered in agile surveillance systems capable of countering adversarial responses. PI Krishnaprasad will present new results at a Northrop Grumman Research Symposium in October 2019.
- **PI Krishnaprasad:** A new collaboration, including joint proposal development has been initiated with Ford in the area of autonomous systems and machine learning.